

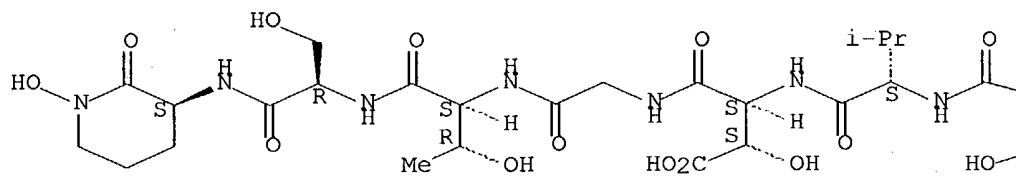
hand note

L14 ANSWER 1 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:239321 CAPLUS Full-text
DN 140:302297
TI Potent Inhibition of Ca²⁺ Release-activated Ca²⁺ Channels and T-lymphocyte Activation by the Pyrazole Derivative BTP2
AU Zitt, Christof; Strauss, Bettina; Schwarz, Eva C.; Spaeth, Nicola; Rast, Georg; Hatzelmann, Armin; Hoth, Markus
CS Department of Physiology, ALTANA Pharma AG, Department of Biochemistry, University of the Saarland, Homburg, 66421, Germany
SO Journal of Biological Chemistry (2004), 279(13), 12427-12437
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
AB Ca²⁺ entry through store-operated Ca²⁺ release-activated Ca²⁺ (CRAC) channels is essential for T-cell activation and proliferation. Recently, it has been shown that 3,5-bistrifluoromethyl pyrazole (BTP) derivs. are specific inhibitors of Ca²⁺-dependent transcriptional activity in T-cells (Trevillyan, J. M., et al., 2001). Whereas inhibition of Ca²⁺ signals was reported for BTP2 (Ishikawa, J., et al., 2003), it was not found for BTP3 (Chen, Y., et al., 2002). We show that BTP2 specifically inhibits CRAC channels in T-cells with an IC₅₀ of .apprx.10 nM. It does not interfere with other mechanisms important for Ca²⁺ signals in T-cells, including Ca²⁺ pumps, mitochondrial Ca²⁺ signaling, endoplasmic reticulum Ca²⁺ release, and K⁺ channels. BTP2 inhibits Ca²⁺ signals in peripheral blood T-lymphocytes (in particular in CD4⁺ T-cells) and in human Jurkat T-cells. Inhibition of Ca²⁺ signals is independent of the stimulation method as Ca²⁺ entry was blocked following stimulation with anti-CD3, which activates the T-cell receptor, and also following stimulation with thapsigargin or inositol 1,4,5-trisphosphate. BTP2 also inhibited Ca²⁺-dependent gene expression (interleukins 2 and 5 and interferon γ) and proliferation of T-lymphocytes with similar IC₅₀ values. BTP2 is the first potent and specific inhibitor of CRAC channels in primary T-lymphocytes. The inhibition of CRAC channels as well as Ca²⁺-dependent signal transduction with similar IC₅₀ values in T-lymphocytes emphasizes the importance of CRAC channel activity during T-cell activation. Furthermore, BTP2 could prove to be a tool to finally unmask the mol. identity of CRAC channels.
IT **367252-76-4**
RL: BSU (Biological study, unclassified); BIOL (Biological study) (potent inhibition of Ca²⁺ release-activated Ca²⁺ channels and T-lymphocyte activation by the pyrazole derivative BTP2)
RN 367252-76-4 CAPLUS
CN D-Serinamide, N-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-valyl-(3S)-3-hydroxy-L- α -aspartylglycyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

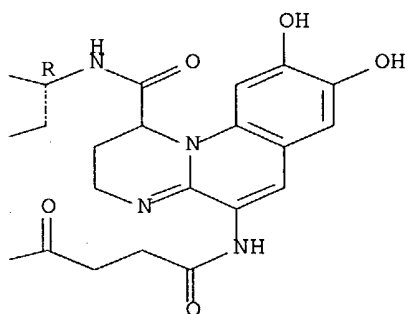
Currently available stereo shown.

PAGE 1-A



H₂N—

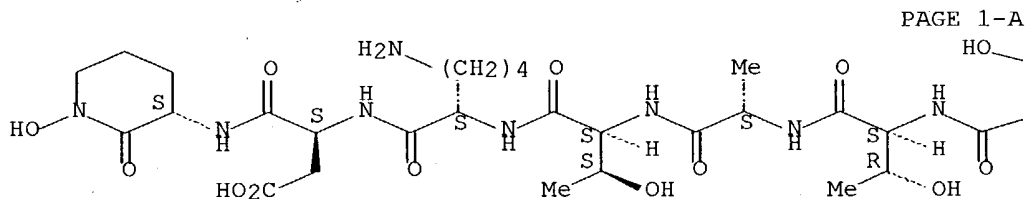
PAGE 1-B

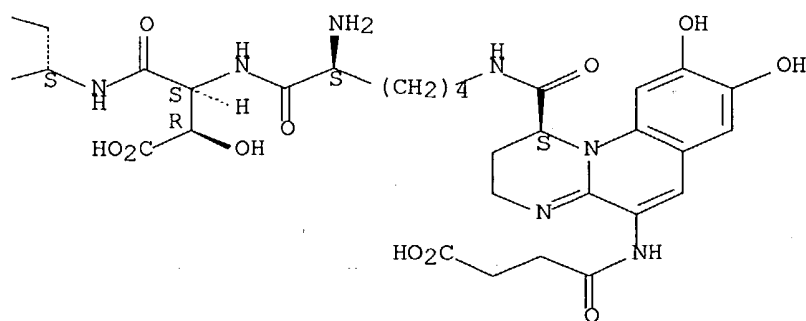


RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2003:781882 CAPLUS Full-text
 DN 141:35164
 TI Bacterial Constituents. CXIII. Structure Revision of Several Pyoverdins Produced by Plant-Growth Promoting and Plant-Deleterious *Pseudomonas* Species
 AU Uria Fernandez, Diana; Geoffroy, Valerie; Schaefer, Mathias; Meyer, Jean-Marie; Budzikiewicz, Herbert
 CS Institut fuer Organische Chemie der Universitaet zu Koeln, Cologne, D-50939, Germany
 SO Monatshefte fuer Chemie (2003), 134(10), 1421-1431
 CODEN: MOCMB7; ISSN: 0026-9247
 PB Springer-Verlag Wien
 DT Journal
 LA English
 AB The structural revision on the basis of spectroscopic and degradation results of several pyoverdins from *Pseudomonas* spp. is reported. Siderotyping studies by the isoelectrofocusing technique and by ferri-pyoverdin uptake expts. had prompted a re-investigation of some structures proposed in the literature.
 IT 701285-45-2 701285-46-3 701285-47-4
 RL: PRP (Properties)
 (structure revision of pyoverdins from plant growth-promoting and plant-deleterious *Pseudomonas* species)
 RN 701285-45-2 CAPLUS
 CN L- α -Asparagine, N6-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-L- α -aspartyl-L-seryl-L-threonyl-L-alanyl-L-allothreonyl-L-lysyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

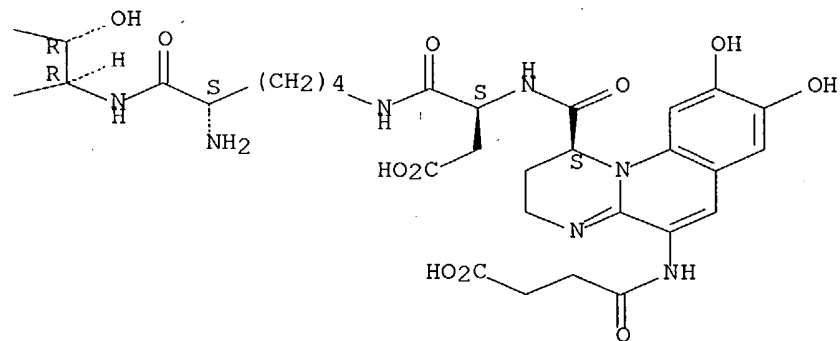
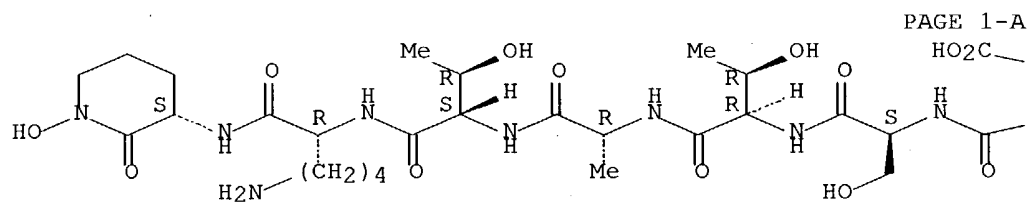




RN 701285-46-3 CAPLUS

CN D-Lysinamide, N6-[N-[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L- α -aspartyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-seryl-D-allothreonyl-D-alanyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

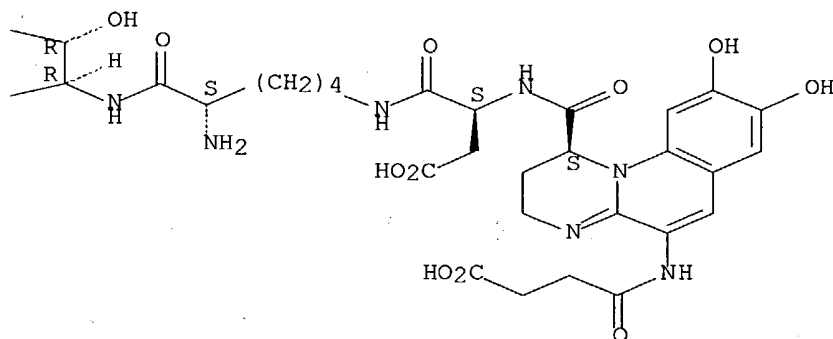
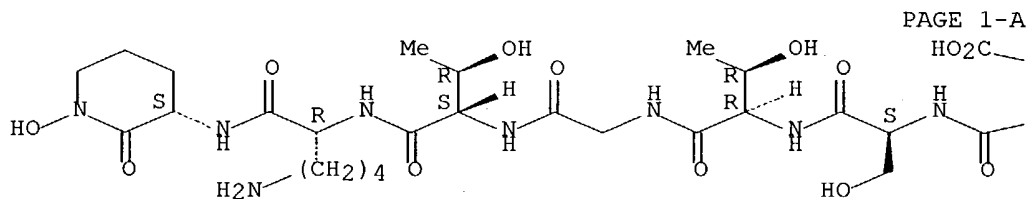
Absolute stereochemistry.



RN 701285-47-4 CAPLUS

CN D-Lysinamide, N6-[N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L- α -aspartyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-seryl-D-allothreonylglycyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2002:209757 CAPLUS Full-text
 DN 136:366203
 TI The structures of the pyoverdins from two *Pseudomonas fluorescens* strains
 accepted mutually by their respective producers
 AU Barelmann, Insa; Taraz, Kambiz; Budzikiewicz, Herbert; Geoffroy, Valerie;
 Meyer, Jean-Marie
 CS Institut fur Organische Chemie der Universitat zu Koln, Koln, 50939, Germany
 SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (2002), 57(1/2), 9-16
 CODEN: ZNCBDA; ISSN: 0939-5075
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB From *Pseudomonas fluorescens* PL7 and PL8 structurally related pyoverdins (I and II) were isolated and their primary structures were elucidated by spectroscopic methods and degradation reactions. Despite of some structural differences, both Fe(III) complexes are taken up by either strain with a high rate. The implications regarding the recognition at the cell surface are discussed.

IT **422563-91-5 422563-93-7**

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(structures of the pyoverdins from two *Pseudomonas fluorescens* strains

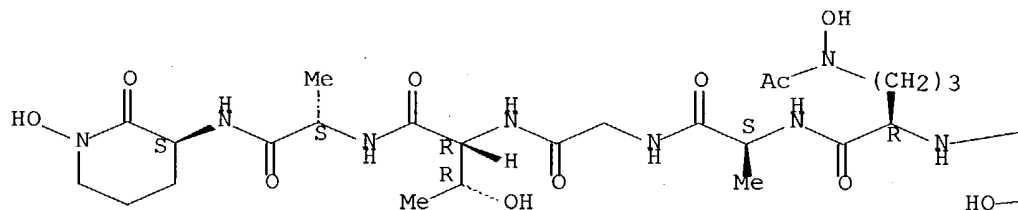
accepted mutually by their resp. producers)

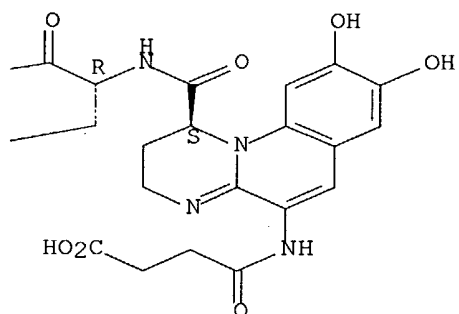
RN 422563-91-5 CAPLUS

CN L-Alaninamide, N-[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-N5-acetyl-N5-hydroxy-D-ornithyl-L-alanylglycyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

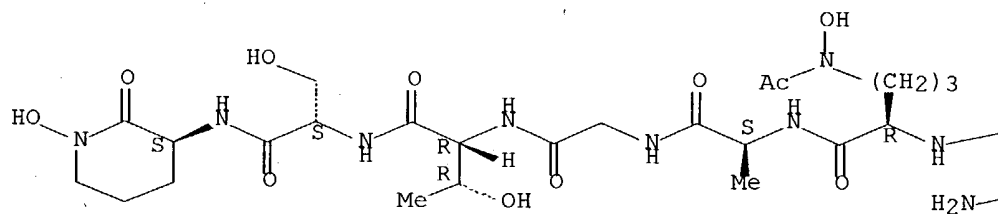
PAGE 1-A

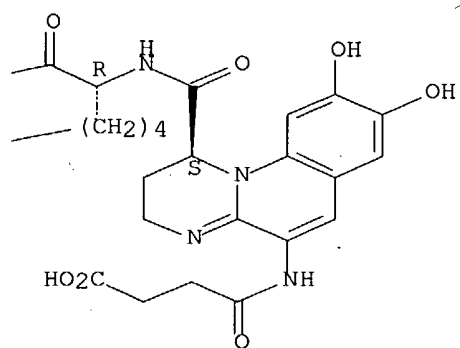




RN 422563-93-7 CAPLUS
 CN L-Serinamide, N2-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-lysyl-N5-acetyl-N5-hydroxy-D-ornithyl-L-alanylglycyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:139736 CAPLUS Full-text

DN 137:59964

TI Unusual traits of the pyoverdinin-mediated iron acquisition system in *Pseudomonas putida* strain BTP1

AU Ongena, Marc; Jacques, Philippe; Delfosse, Philippe; Thonart, Philippe

CS Centre Wallon de Biologie Industrielle, Unite de Bio-industries, Unite de

Gembloux, Bio-industries, Faculte Universitaire des Sciences Agronomiques, B-5030, Belg.

SO BioMetals (2002), 15(1), 1-13
CODEN: BOMEHH; ISSN: 0966-0844

PB Kluwer Academic Publishers

DT Journal

LA English

AB Fluorescent *Pseudomonas* species are characterized by the production of pyoverdinin-type siderophores for Fe³⁺ acquisition in iron-limited environments. Since it produces a structurally specific pyoverdinin, *Pseudomonas putida* strain BTP1 could represent a valuable tool in an attempt to correlate the structural features of these compds. with some specificity in their two main properties i.e. affinity for iron and recognition rate by other *Pseudomonas* strains. An uncommonly high affinity for iron of the pyoverdinin synthesized by *P. putida* BTP1 was observed by comparing both the apparent stability constant and the decomplexation kinetics of its ferric complex with those of ferripyoverdins from other strains. IROMP. On another hand, results from growth stimulation expts. and labeled ferripyoverdinin uptake assays highlighted the very low recognition rate of BTP1 isopyoverdins by membrane receptors of foreign strains. By contrast, *P. putida* BTP1 was able to utilize a broad spectrum of structurally unrelated exogenous pyoverdins by means of multiple receptors that are likely constitutively expressed in its outer membrane. The unusual traits of its pyoverdinin-mediated iron acquisition system should contribute to enlarge the ecol. competence of *Pseudomonas putida* BTP1 in terms of colonization and persistence in the rhizosphere.

IT 439660-57-8D, Pyoverdinin BTP2, iron complexes

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

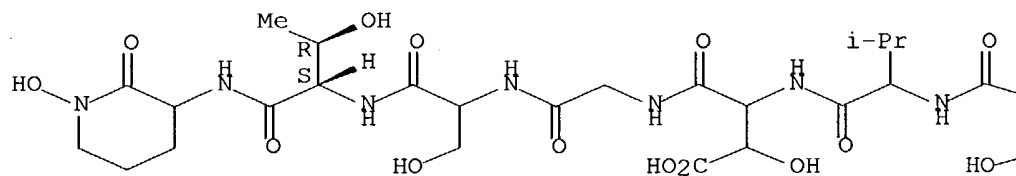
(stability consts. of ferric complexes of pyoverdins from *Pseudomonas putida* BTP1 and other strains)

RN 439660-57-8 CAPLUS

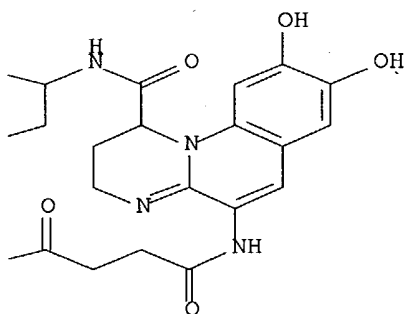
CN Threoninamide, N-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]serylvalyl-3-hydroxy- α -aspartylglycylseryl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Currently available stereo shown.

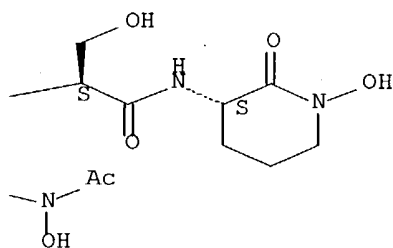
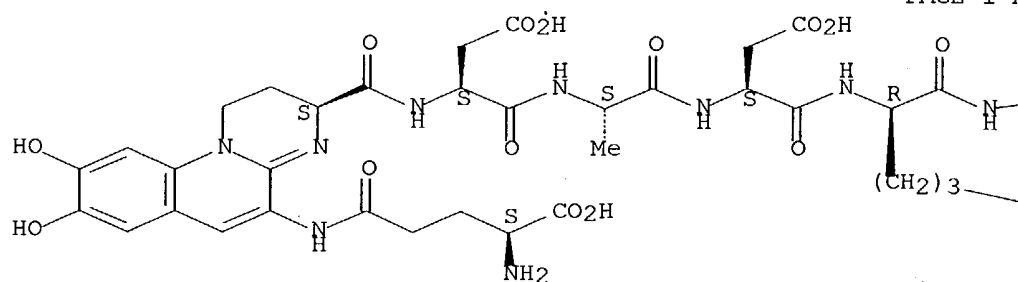


H2N—



IT 159325-01-6 159325-01-6D, iron complexes
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
 (Biological study)
 (unusual traits of the pyoverdinin-mediated iron acquisition system in
 Pseudomonas putida strain BTP1)
 RN 159325-01-6 CAPLUS
 CN L-Serinamide, L-γ-glutamyl-(3S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-
 pyrimido[1,2-a]quinoline-3-carbonyl-L-α-aspartyl-L-alanyl-L-α-
 aspartyl-N5-acetyl-N5-hydroxy-D-ornithyl-N-[(3S)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

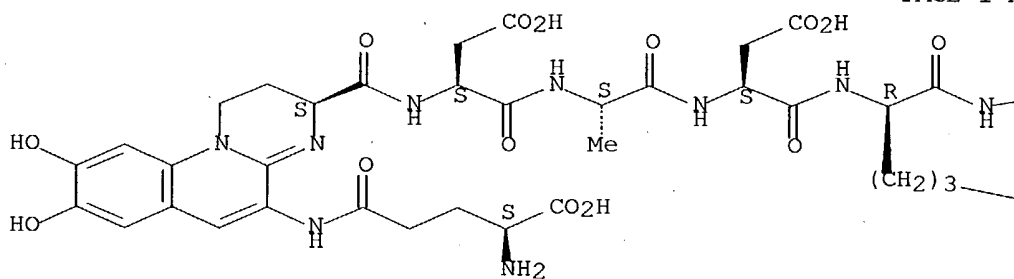
Absolute stereochemistry.

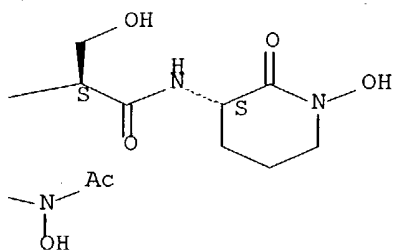


RN 159325-01-6 CAPLUS

CN L-Serinamide, L-γ-glutamyl-(3S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinoline-3-carbonyl-L-α-aspartyl-L-alanyl-L-α-aspartyl-N5-acetyl-N5-hydroxy-D-ornithyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



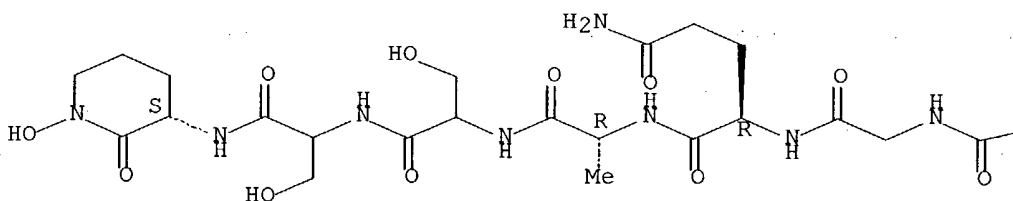


RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

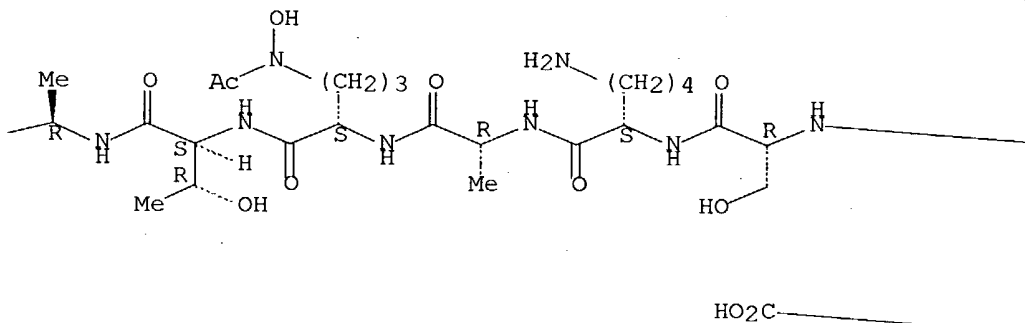
L14 ANSWER 5 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:746828 CAPLUS Full-text
 DN 136:167659
 TI Rearrangement reactions in the electrospray ionization mass spectra of pyoverdins
 AU Fuchs, Regine; Budzikiewicz, Herbert
 CS Institut für Organische Chemie der Universität zu Köln, Cologne, 50939, Germany
 SO International Journal of Mass Spectrometry (2001), 210/211(1-3), 603-612
 CODEN: IMSPF8; ISSN: 1387-3806
 PB Elsevier Science B.V.
 DT Journal
 LA English
 AB The electrospray ionization mass spectra of pyoverdins, chromopeptidic siderophores of the bacterial family Pseudomonas, especially when analyzed by collision activation in an ion trap, show rearrangement reactions which can lead to erroneous structure proposals. Several of these processes will be described.
 IT **292840-54-1**
 RL: PRP (Properties)
 (rearrangement reactions in the electrospray ionization mass spectra of pyoverdins)
 RN 292840-54-1 CAPLUS
 CN Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-D-alanyl-N5-acetyl-N5-hydroxy-L-ornithyl-L-threonyl-D-alanylglycyl-D-glutamyl-D-alanylseryl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

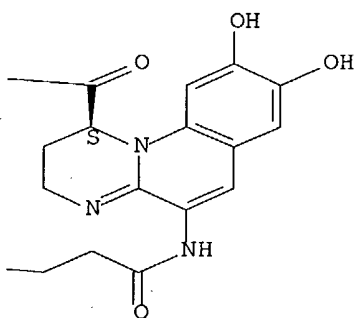
Absolute stereochemistry.
 Currently available stereo shown.

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RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 6 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:731047 CAPLUS Full-text

DN 135:283965

TI Methods of preparing recombinant neisserial iron uptake proteins and uses as a vaccine

IN Gorringer, Andrew Richard; Hudson, Michael John; Matheson, Mary Anne; Robinson, Andrew; West, David McKay

PA Microbiological Research Authority, UK

SO PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001073080	A2	20011004	WO 2001-GB1348	20010327
	WO 2001073080	A3	20020214		
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	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 2001044311	A5	20011008	AU 2001-44311	20010327
	EP 1268822	A2	20030102	EP 2001-917226	20010327
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003528615	T2	20030930	JP 2001-570797	20010327
	US 2003186848	A1	20031002	US 2003-240218	20030424
PRAI	GB 2000-7433	A	20000327		
	WO 2001-GB1348	W	20010327		

AB The invention discloses methods of making recombinant neisserial iron uptake proteins including transferrin binding protein A (TbpA) and B (TbpB) in both full length form and uses as immunogenic fragments for vaccination. In particular, the invention discloses that a non-neisserial cell expresses TbpA or TbpB which is located on or associated with the cell surface, hence it can be extracted under mild conditions and retains substantially the antigenicity of native TbpA or TbpB on its surface. The invention further provides methods to express both recombinant TbpA and TbpB in the same cell as well as the expression cassettes, host cells and methods of protein purification. The invention discloses that TbpA and TbpB are antigenic and stimulates an immune response against Tbp and organisms expressing Tbp in animal models. The invention further provides applications of the proteins as a vaccine against neisserial infection.

IT 76975-04-7, pseudobactin

RL: BSU (Biological study, unclassified); BIOL (Biological study)

(binding protein; methods of preparing recombinant neisserial iron uptake proteins and uses as a vaccine)

RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

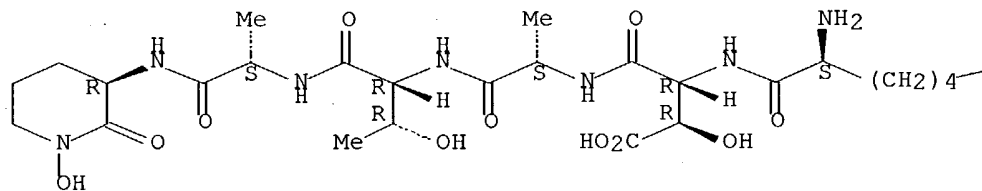
dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

hydroxy-

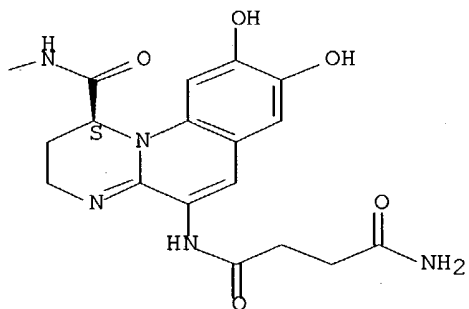
D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



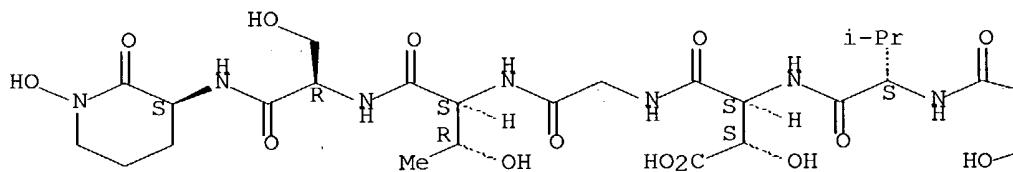
PAGE 1-B



L14 ANSWER 7 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:557687 CAPLUS Full-text
 DN 135:300774
 TI The pyoverdinin of *Pseudomonas fluorescens* BTP2, a novel structural type
 AU Ongena, M.; Jacques, P.; Thonart, P.; Gwose, I.; Fernandez, D. U.;
 Schafer, M.; Budzikiewicz, H.
 CS Centre Wallon de Biologie Industrielle, Universite de Liege, Liege,
 4000, Belg.
 SO Tetrahedron Letters (2001), 42(34), 5849-5851
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 AB From *Pseudomonas fluorescens* BTP2 a pyoverdinin was isolated which
 contained valine in its peptide chain. Its structure could be
 elucidated by chemical degradation and spectroscopic data.
 IT **367252-76-4P**
 RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP
 (Properties); PUR (Purification or recovery); BIOL (Biological study);
 FORM (Formation, nonpreparative); PREP (Preparation)
 (pyoverdinin of *Pseudomonas fluorescens* BTP2, novel structural type)
 RN 367252-76-4 CAPLUS
 CN D-Serinamide, N-[[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-valyl-
 (3S)-3-hydroxy-L- α -aspartylglycyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

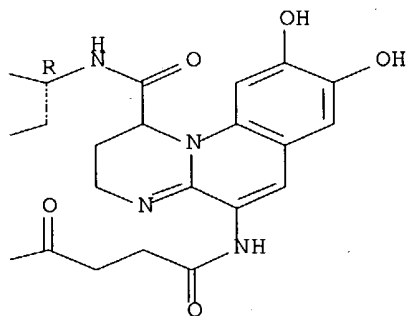
Absolute stereochemistry.
 Currently available stereo shown.

PAGE 1-A



H₂N

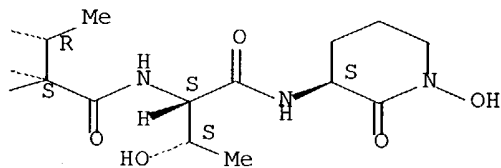
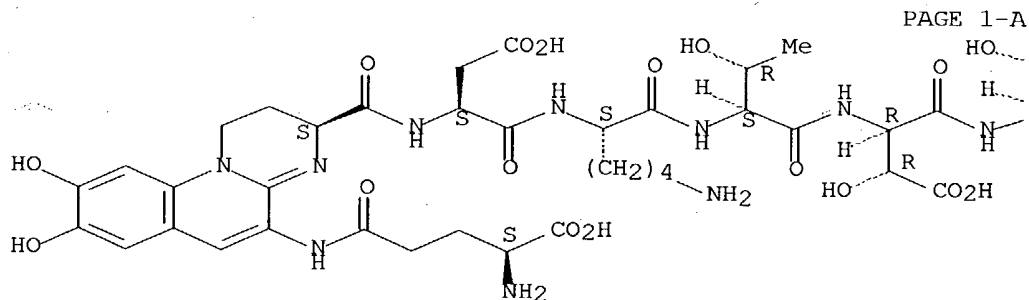
PAGE 1-B



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD

L14 ANSWER 9 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:83711 CAPLUS Full-text
 DN 134:292465
 TI An isopyoverdin from *Pseudomonas putida* CFML 90-33
 AU Sultana, R.; Siddiqui, B. S.; Taraz, K.; Budzikiewicz, H.; Meyer, J.-M.
 CS Institut für Organische Chemie der Universität zu Köln, Köln, D-50939,
 Germany
 SO Tetrahedron (2001), 57(6), 1019-1023
 CODEN: TETRAB; ISSN: 0040-4020
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 AB An isopyoverdin was isolated from *Pseudomonas putida* CFML 90-33.
 The structure elucidation of this rare variety of siderophore of
 fluorescent pseudomonads is described.
 IT **334009-11-9P**
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 PRP
 (Properties); PUR (Purification or recovery); BIOL (Biological study);
 OCCU (Occurrence); PREP (Preparation)
 (isopyoverdin from *Pseudomonas putida* CFML 90-33)
 RN 334009-11-9 CAPLUS
 CN L-Allothreoninamide, L-γ-glutamyl-(3S)-5-amino-2,3-dihydro-8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinoline-3-carbonyl-L-α-aspartyl-L-
 lysyl-L-threonyl-(3R)-3-hydroxy-D-α-aspartyl-L-threonyl-N-[(3S)-1-
 hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

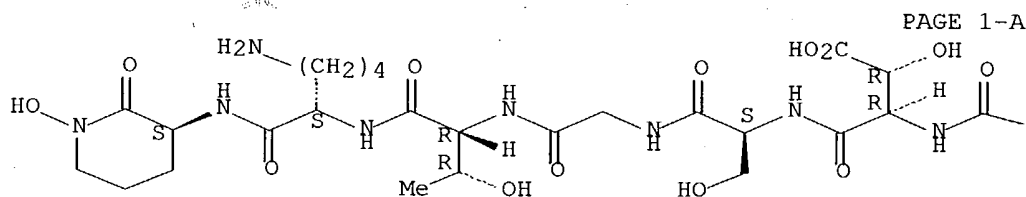
Absolute stereochemistry.



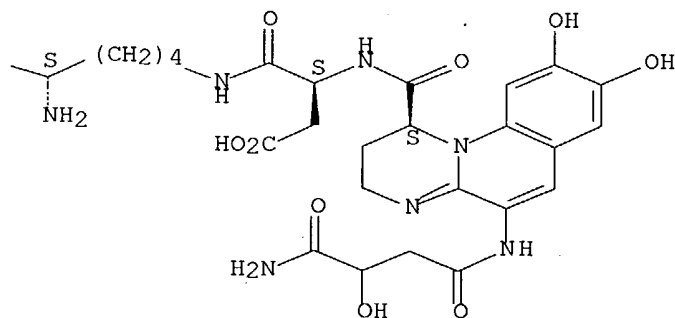
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2000:696113 CAPLUS Full-text
 DN 134:15003
 TI A pyoverdine from *Pseudomonas putida* CFML 90-51 with a Lys ϵ -amino link in the peptide chain
 AU Sultana, Razia; Siddiqui, Bina Shaheen; Taraz, Kambiz; Budzikiewicz, Herbert; Meyer, Jean-Marie
 CS Institut für Organische Chemie der Universität zu Köln, Köln, 50939, Germany
 SO BioMetals (2000), 13(2), 147-152
 CODEN: BOMEEH; ISSN: 0966-0844
 PB Kluwer Academic Publishers
 DT Journal
 LA English
 AB From *Pseudomonas putida* CFML 90-51, a hospital isolate, a pyoverdine was obtained which is characterized by the unusual linkage by the ϵ -rather than the α -amino group of Lys in the peptide chain. Structure elucidation by spectroscopic methods and degradation reactions are reported.
 IT **309759-53-3**
 RL: PRP (Properties)
 (pyoverdine from *Pseudomonas putida* CFML 90-51 with a Lys ϵ -amino link in the peptide chain)
 RN 309759-53-3 CAPLUS
 CN L-Lysinamide, N6-[N-[[[(1S)-5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L- α -aspartyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-serylglycyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Currently available stereo shown.



PAGE 1-B

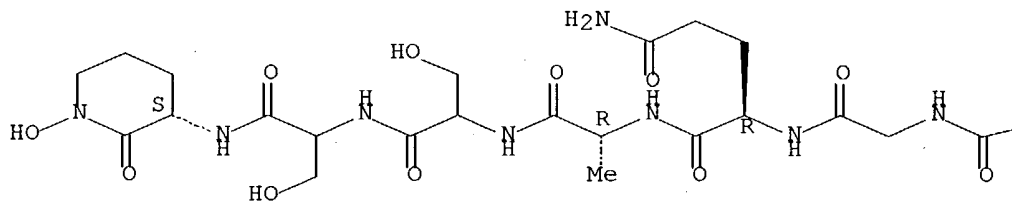


RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

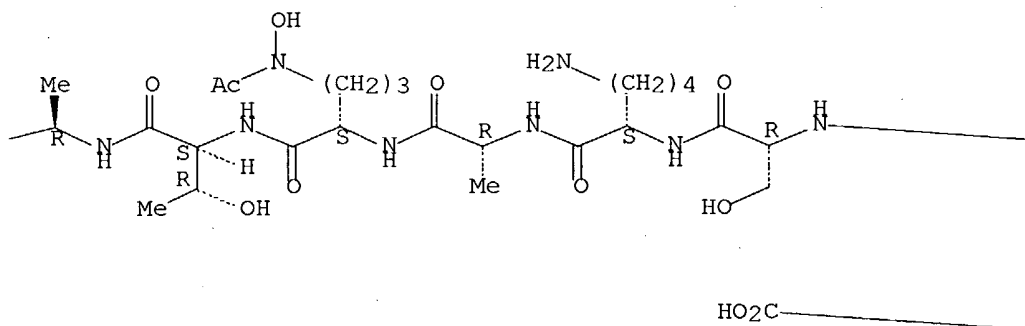
L14 ANSWER 11 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2000:505324 CAPLUS Full-text
 DN 133:234852
 TI Bacterial constituents. Part LXXXVIII. An exceptionally large pyoverdin from a Pseudomonas strain collected in Thailand
 AU Ruangviriyachai, Chalerm; Barelmann, Insa; Fuchs, Regine; Budzikiewicz, Herbert
 CS Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen, 40002, Thailand
 SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (2000), 55(5/6), 323-327
 CODEN: ZNCBDA; ISSN: 0939-5075
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 AB From a Pseudomonas strain obtained from a soil sample collected in Thailand a pyoverdin was obtained that contained twelve amino acids in its peptide chain. The structure elucidation is described.
 IT **292840-54-1P**, Pyoverdin Pf 1547
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (exceptionally large pyoverdin from Pseudomonas collected in Thailand)
 RN 292840-54-1 CAPLUS
 CN Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-D-alanyl-N5-acetyl-N5-hydroxy-L-ornithyl-L-threonyl-D-alanylglycyl-D-glutamyl-D-alanylseryl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.
 Currently available stereo shown.

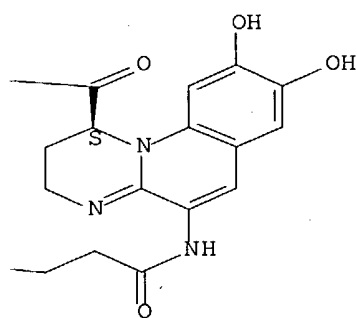
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PAGE 1-B



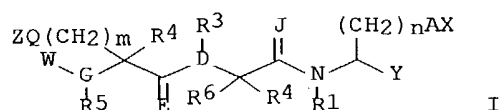
PAGE 1-C



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 12 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2000:219109 CAPLUS Full-text
 DN 132:251428
 TI Preparation of peptidyl inhibitors of factor Xa for treatment of
 coagulation disorders
 IN Marlowe, Charles K.; Scarborough, Robert M.; Laibelman, Alan M.; Sinha,
 Uma; Zhu, Bing-Yan
 PA COR Therapeutics, Inc., USA
 SO U.S., 26 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6046169	A	20000404	US 1995-486386	19950607
PRAI	US 1995-486386		19950607		
OS	MARPAT 132:251428				
GI					



AB Novel compds. I [m, n = 0-4; Y = CHO, COCF₃, COCF₂CF₃, etc.; A = absent, piperidinyl, pyrrolidinyl, cyclopropyl, Ph, etc.; R₁, R₂, R₃ = H, alkyl; R₄ = H, Me; J, E = O, H₂; D = N, CH, NCH₂, NCH₂CH₂, CHCH₂; Q = absent, piperidinyl, pyrrolidinyl, cycloalkyl, Ph, naphthyl, pyridyl, etc.; G = N, CH, H; R₅ = H, alkyl, or absent; R₆ = H, Me; W = absent, H, arylacyl, heteroarylacyl, arylsulfonyl, alkylaminocarbonyl, etc.; X, Z = NR'R'', NHC(NR'R'') : NH, NHC(NR'R'') : NR'', SC(NR'R'') : NH, etc. (R' and R'' are H, alkyl, arylalkyl, aryl or R'R'' is alkylene)] or their pharmaceutically acceptable salts, prodrugs, etc. were prepared as factor Xa inhibitors. The compds. are useful in vitro or in vivo for preventing or treating coagulation disorders. Thus, Boc-D-Arg-Gly-Arg-H (Boc = tert-butoxycarbonyl) was prepared by reduction-hydrogenolysis of Boc-D-Arg(Cbz₂)-Gly-Arg(N-Cbz)-lactam (Cbz = benzyloxycarbonyl), which was prepared by peptide coupling in solution. The product was evaluated in rabbits for biol. half-life, antithrombotic efficacy, and effects on hemostasis and hematol. parameters.

IT **186369-07-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT

(Reactant or reagent)

(preparation of peptidyl inhibitors of factor Xa for treatment of
 coagulation disorders)

RN 186369-07-3 CAPLUS

CN Glycinamide, N2-[1,4-dioxo-4-(phenylmethoxy)butyl]-N5-

[imino[(phenylmethoxy)carbonyl]amino]methyl]-N5-

[(phenylmethoxy)carbonyl]-

D-orithyl-N-[(3S)-1-[imino[(phenylmethoxy)carbonyl]amino]methyl]-2-

oxo-3-

piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

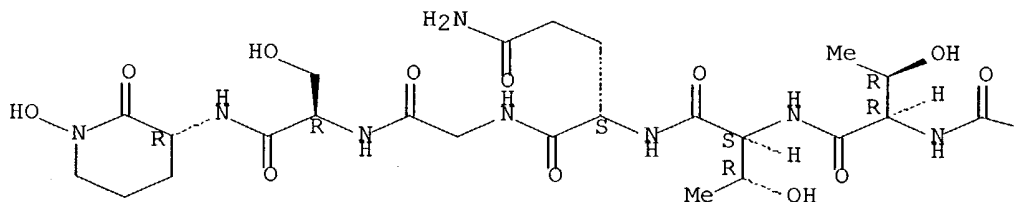
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$$\text{---} \text{---} \text{Ph}$$

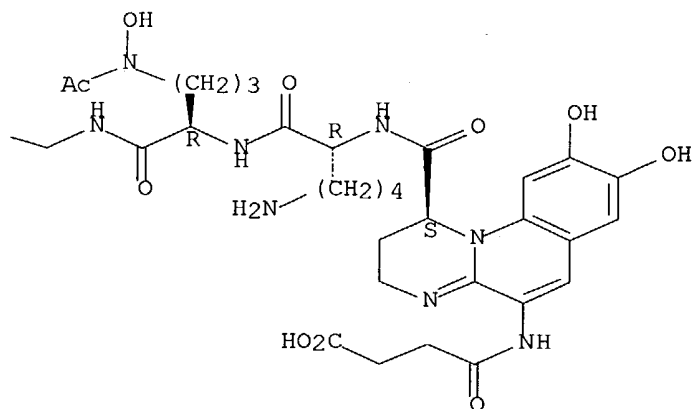
RE.CNT 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 13 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2000:208945 CAPLUS Full-text
 DN 133:30927
 TI Revised structures of the pyoverdins from *Pseudomonas putida* CFBP 2461
 and
 from *Pseudomonas fluorescens* CFBP 2392
 AU Beiderbeck, H.; Taraz, K.; Meyer, J.-M.
 CS Institut fur Organische Chemie der Universitat zu Koln, Koln, D-50939,
 Germany
 SO BioMetals (2000), Volume Date 1999, 12(4), 331-338
 CODEN: BOMEEH; ISSN: 0966-0844
 PB Kluwer Academic Publishers
 DT Journal
 LA English
 AB Several suggestions for structures of the siderophores (pyoverdins) from
Pseudomonas spp. can be found in the literature which are based on a FAB
 mass spectrometric anal. only. Availability of two original strains of
 two *Pseudomonas* spp. allowed reinvestigation of the structure of their
 pyoverdins. In both cases the amino acid sequence had to be corrected.
 In addition, D- and L-amino acids could be identified and located in the
 peptide chain. The knowledge of the correct structures is important in
 view of an ongoing study to establish relationships between the nature
 of the peptide chains of pyoverdins and their recognition by outer
 membrane proteins.
 IT 273378-29-3
 RL: PRP (Properties)
 (revised structure of pyoverdin from *Pseudomonas fluorescens* CFBP
 2392)
 RN 273378-29-3 CAPLUS
 CN D-Serinamide, N2-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-lysyl-N5-acetyl-
 N5-
 hydroxy-D-ornithylglycyl-D-allothreonyl-L-threonyl-L-glutaminylglycyl-N-
 [(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





IT 273378-27-1 273378-28-2

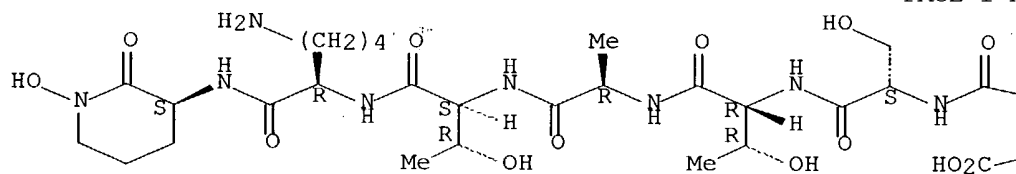
RL: PRP (Properties)

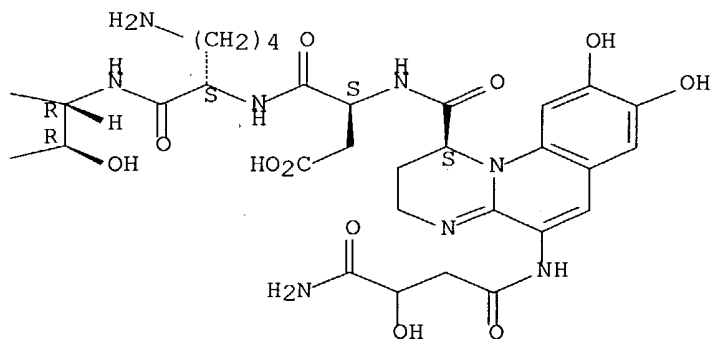
(revised structure of pyoverdin from *Pseudomonas putida* CFBP 2461)

RN 273378-27-1 CAPLUS

CN D-Lysinamide, N-[[[(1S)-5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-α-aspartyl-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-seryl-D-allothreonyl-D-alanyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



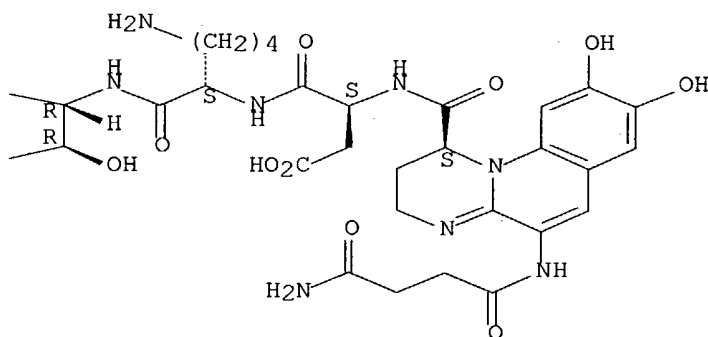
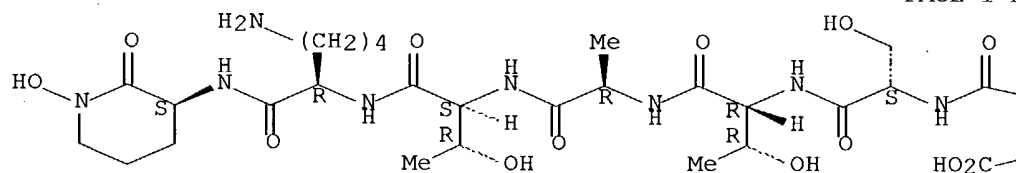


RN 273378-28-2 CAPLUS

CN D-Lysinamide, N-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L- α -aspartyl-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-seryl-D-allothreonyl-D-alanyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

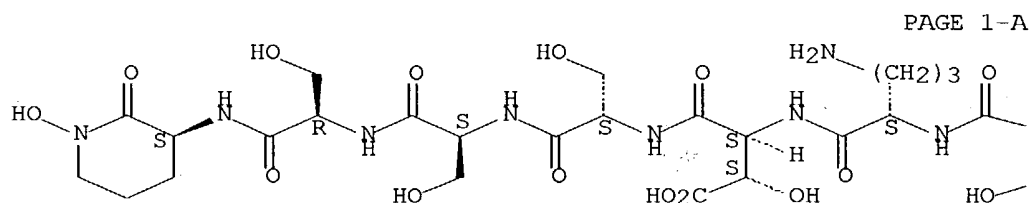
Absolute stereochemistry.



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

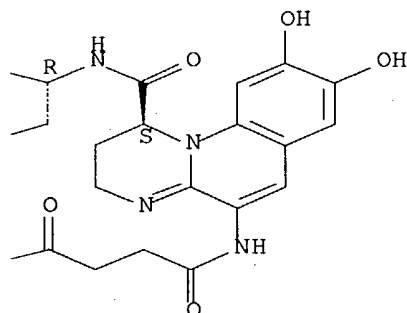
L14 ANSWER 14 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2000:208944 CAPLUS Full-text
 DN 133:2296
 TI Structure of the pyoverdin PVD 2908 - a new pyoverdin from *Pseudomonas*
 sp. 2908
 AU Vossen, W.; Taraz, K.
 CS Institut für Organische Chemie der Universität zu Köln, Köln, D-50939,
 Germany
 SO BioMetals (2000), Volume Date 1999, 12(4), 323-329
 CODEN: BOMEHH; ISSN: 0966-0844
 PB Kluwer Academic Publishers
 DT Journal
 LA English
 AB An unknown siderophore (pyoverdin) was isolated from the strain
Pseudomonas sp. 2908. The structure of the pyoverdin - called PVD 2908
 - was elucidated by spectroscopic methods and degradation studies. Some
 other siderophores were identified by LC/ESI-MS-screening based on the
 knowledge of PVD 2908.
 IT **270251-13-3P**, Pyoverdin PVD 2908
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 PRP (Properties); PUR (Purification or recovery); BIOL (Biological
 study); OCCU (Occurrence); PREP (Preparation) (structure of the new
 pyoverdin PVD 2908 from *Pseudomonas* 2908)
 RN 270251-13-3 CAPLUS
 CN Pyoverdin PVD 2908 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HO₂C—

PAGE 1-B



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 15 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:119589 CAPLUS Full-text

DN 132:290807

TI Bacterial constituents. Part LXXXV. Pyoverdins with a Lys ϵ -amino link in the peptide chain?

AU Budzikiewicz, Herbert; Fernandez, Diana Uria; Fuchs, Regine; Michalke, Roland; Taraz, Kambiz; Rungiviriachai, Chalerm

CS Institut fur Organische Chemie der Universitat zu Koln, Koln, 50939, Germany

SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1999), 54(12),

1021-1026

CODEN: ZNCBDA; ISSN: 0939-5075

PB Verlag der Zeitschrift fuer Naturforschung

DT Journal

LA English

AB For a pyoverdin isolated from *Pseudomonas putida* it could be shown that Lys is incorporated into the peptide chain by its ϵ -amine group in contrast to the normally observed connection by the α -amino group. The structure elucidation of the pyoverdin by chemical degradation and spectroscopic methods is reported and the criteria for the distinction between α - and ϵ -connection in the case of Lys are discussed.

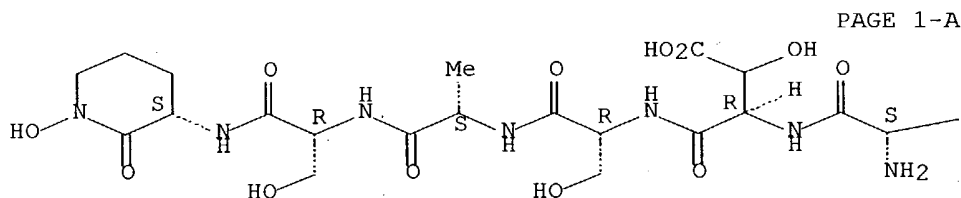
IT **264189-47-1P**

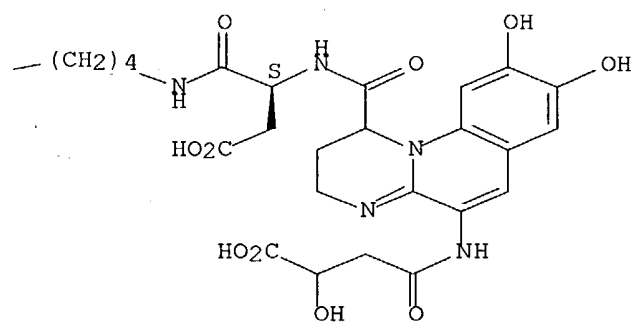
RL: PRP (Properties); PUR (Purification or recovery); PREP (Preparation)
(lysine is incorporated by ϵ -amino group into peptide chain of pyoverdin from *Pseudomonas putida*)

RN 264189-47-1 CAPLUS

CN D-Serinamide, N6-[N-[[5-[(3-carboxy-3-hydroxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L- α -aspartyl]-L-lysyl-3-hydroxy-D- α -aspartyl-D-seryl-L-alanyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 16 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:53681 CAPLUS Full-text

DN 132:108302

TI Preparation of CS-1 peptidomimetics and their compositions

IN Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.; He, Ya-Bo; Huyghe, Bernard G.; Chen, Paul G.

PA Cytel Corporation, USA

SO PCT Int. Appl., 266 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000002903	A1	20000120	WO 1998-US26605	19981215
	W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,			

TM

RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

	AU 9919153	A1	20000201	AU 1999-19153	19981215
PRAI	US 1998-113689		19980710		
	WO 1998-US26605		19981215		

OS MARPAT 132:108302

AB Peptidomimetics R1CONR2CHR3CONR4CH(CONR5R6)CH2CO2H [R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, alkyl, phenylalkyl or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl, dialkyl thioether, or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, an optionally substituted 5-, 6-, or 7-membered heterocyclic ring containing 1 or 2 nitrogen atoms, a pyridobenzazepine moiety, or a group CHR7CO-AR8R9 (A = N and R7, R8, R9 = alkyl, a ring structure, etc. or A = O and R7 = alkyl, a ring structure, etc., R8 = alkyl, and R9 is absent)] were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-L-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

IT **209601-18-3P 209601-35-4P 209601-64-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

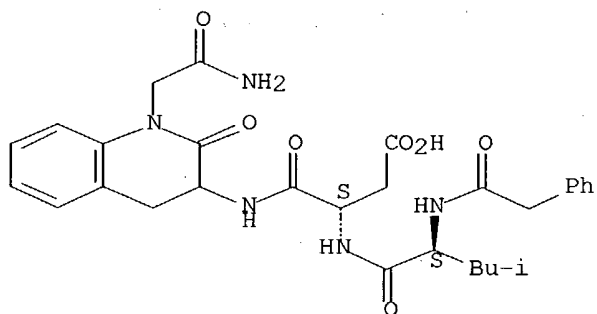
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of CS-1 peptidomimetics and their compns.)

RN 209601-18-3 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1-(2-amino-2-oxoethyl)-1,2,3,4-tetrahydro-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

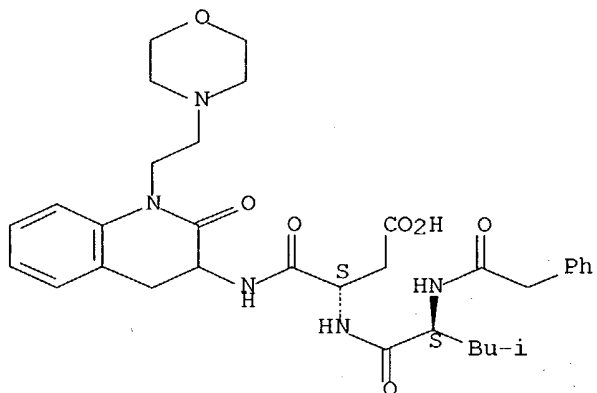
Absolute stereochemistry.



RN 209601-35-4 CAPLUS

CN L-α-Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-[2-(4-morpholinyl)ethyl]-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

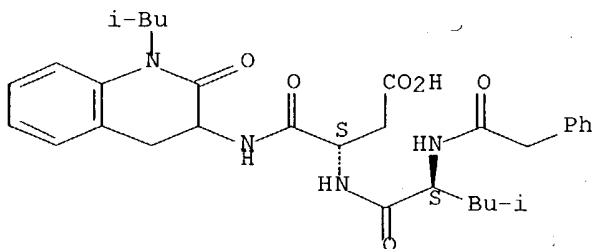
Absolute stereochemistry.



RN 209601-64-9 CAPLUS

CN L-α-Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-(2-methylpropyl)-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

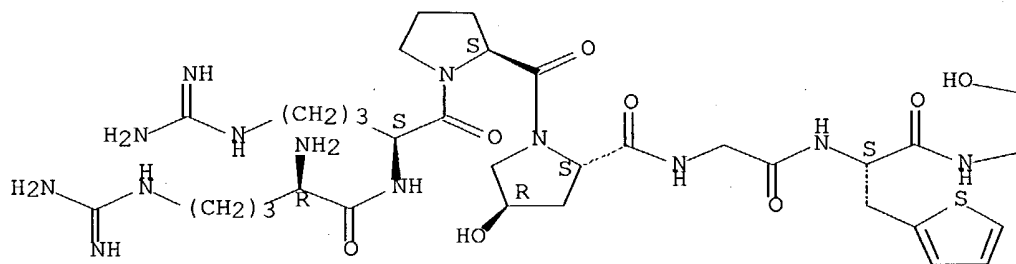


RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

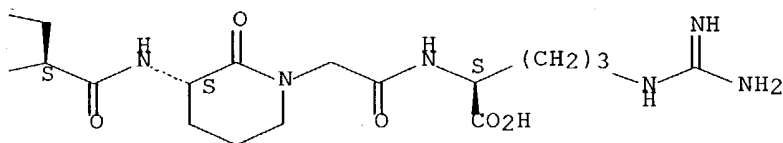
L14 ANSWER 17 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1999:596173 CAPLUS Full-text
 DN 132:3544
 TI Synthesis and Characterization of Bradykinin B2 Receptor Agonists
 Containing Constrained Dipeptide Mimics
 AU Amblard, Muriel; Daffix, Isabelle; Berge, Gilbert; Calmes, Monique;
 Dodey,
 Pierre; Pruneau, Didier; Paquet, Jean-Luc; Luccarini, Jean-Michel;
 Belichard, Pierre; Martinez, Jean
 CS Laboratoire des Aminoacides Peptides et Proteines, Universites
 Montpellier
 I et II Faculte de Pharmacie, Montpellier, 34060, Fr.
 SO Journal of Medicinal Chemistry (1999), 42(20), 4193-4201
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 AB We have previously shown that substitution of the D-Tic-Oic dipeptide by
 a (3S)-[amino]-5-(carbonylmethyl)-2,3-dihydro-1,5-benzothiazepin-4(5H)-
 one (D-BT) moiety in the bradykinin B2 receptor antagonist HOE 140
 resulted in a full potent and selective bradykinin B2 receptor agonist
 (H-DArg-Arg-Pro-Hyp-Gly-Thi-Ser-D-BT-Arg-OH, JMV 1116) exhibiting a high
 affinity for the human receptor (K_i 0.7 nM). In the present study, we
 have investigated the effects of replacement of the D-Tic-Oic moiety by
 various constrained dipeptide mimetics. The resulting compds. were
 tested for their binding affinity toward the cloned human B2 receptor
 and for their functional interaction with the bradykinin-induced
 contraction of isolated human umbilical vein. Subsequently, we have
 designed novel bradykinin B2 receptor agonists which are likely to be
 resistant to enzymic cleavage by endopeptidases and which might
 represent interesting new pharmacol. tools. In an attempt to increase
 the potency of compound JMV 1116, both its N-terminal part and the D-BT
 moiety were modified. Substitution of the D-arginine residue by a L-
 lysine residue led to a 10-fold more potent bradykinin B2 ligand
 [compound JMV 1465 (K_i 0.07 nM)], retaining full agonist activity on
 human umbilical vein. Substitution of the D-BT moiety by a (3S)-[amino]-
 5-(carbonylmethyl)-2,3- dihydro-8-methyl-1,5-benzothiazepin-4(5H)-one
 [D-BT(Me)] moiety led to compound JMV 1609 which exhibited a higher
 agonist activity (pD₂ = 7.4) than JMV 1116 (pD₂ = 6.8).
 IT **250682-64-5P**
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (preparation, binding affinity, functional interaction of bradykinin
 B2
 analogs and bradykinin B2 receptor agonists containing constrained
 dipeptide mimics)
 RN 250682-64-5 CAPLUS
 CN L-Arginine, D-arginyl-L-arginyl-L-prolyl-(4R)-4-hydroxy-L-prolylglycyl-
 3-
 (2-thienyl)-L-alanyl-L-seryl-(3S)-3-amino-2-oxo-1-piperidineacetyl-
 (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 18 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:505686 CAPLUS Full-text

DN 131:139496

TI Fibronectin CS-1 peptidomimetics for inhibiting binding of CS-1 to VLA-4 and for treating immunoinflammatory conditions

IN Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.

PA Cytel Corporation, USA

SO U.S., 81 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5936065	A	19990810	US 1995-462424	19950605
	CA 2177840	AA	19950615	CA 1994-2177840	19941205
	CN 1142832	A	19970212	CN 1994-194969	19941205
	US 5688913	A	19971118	US 1995-435286	19950505
	US 6117840	A	20000912	US 1997-837154	19970414
	US 6103870	A	20000815	US 1997-923026	19970903
PRAI	US 1993-164101	B2	19931206		
	US 1994-349024	B2	19941202		
	US 1995-435286	A1	19950505		

OS MARPAT 131:139496

AB Peptidomimetic compds. are disclosed that inhibit the binding between the VLA-4 and the fibronectin CS-1 compound Pharmaceutical compns. containing a contemplated compound and methods for treating immunoinflammatory conditions using the compound are also disclosed.

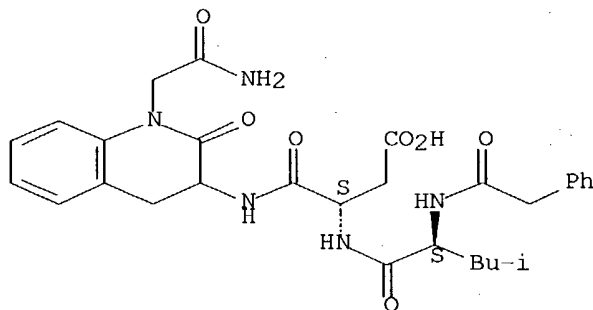
IT **209601-18-3 209601-35-4 209601-64-9**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (fibronectin CS-1 peptidomimetics for inhibiting binding of CS-1 to VLA-4 and for treating immunoinflammatory conditions)

RN 209601-18-3 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1-(2-amino-2-oxoethyl)-1,2,3,4-tetrahydro-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

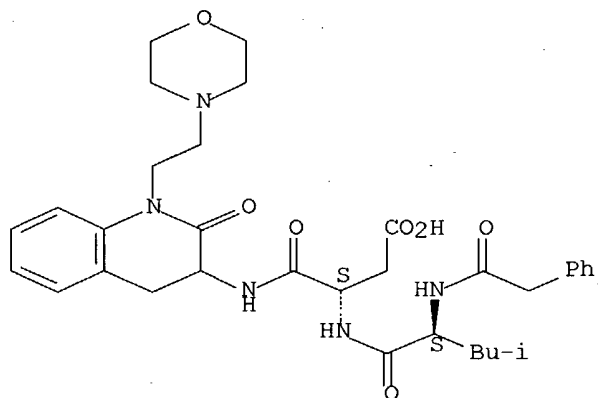
Absolute stereochemistry.



RN 209601-35-4 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-[2-(4-morpholinyl)ethyl]-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

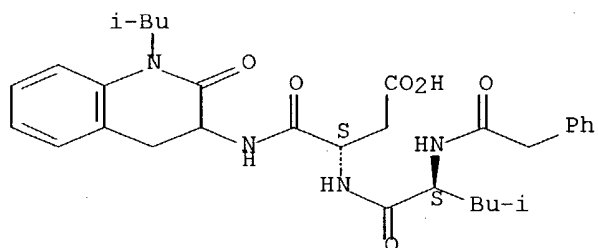
Absolute stereochemistry.



RN 209601-64-9 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-(2-methylpropyl)-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 19 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:347823 CAPLUS Full-text

DN 131:155477

TI Assignment of the absolute configuration of the amino acids of pyoverdins

by GC/MS

AU Dallakian, Paul; Voss, Jessica; Budzikiewicz, Herbert

CS Institut für Organische Chemie, Universität zu Köln, Köln, D-50939, Germany

SO Chirality (1999), 11(5/6), 381-386

CODEN: CHRLEP; ISSN: 0899-0042

PB Wiley-Liss, Inc.

DT Journal

LA English

AB Bacterial peptides frequently contain both D- and L-amino acids, proteinogenic as well as uncommon ones. Using the example of pyoverdins, iron chelating chromopeptides of the bacterial genus *Pseudomonas*, the mass spectrometric assignment of enantiomers of the amino acids in the form of their N(O, S)-perfluoroacyl amino acid alkyl esters after GC separation using a Permabond L-Chirasil Val chiral column is discussed. The identification of the amino acids with different fragmentation patterns is demonstrated even in cases of unresolved peaks by mass spectrometry. A simplified assignment of absolute configuration of the amino acids in low or trace concns. by mass fragmentog. is presented. Although mainly the trifluoroacetyl amino acid iso-Pr ester (TFA-IP derivs.) are used for the anal. of pyoverdins, also other N(O, S)-perfluoroacyl alkyl esters can be used due to reliability and enhanced identification power of GC/MS.

IT 235101-93-6 235101-94-7

RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)

(assignment of absolute configuration of amino acids of pyoverdins by GC/MS)

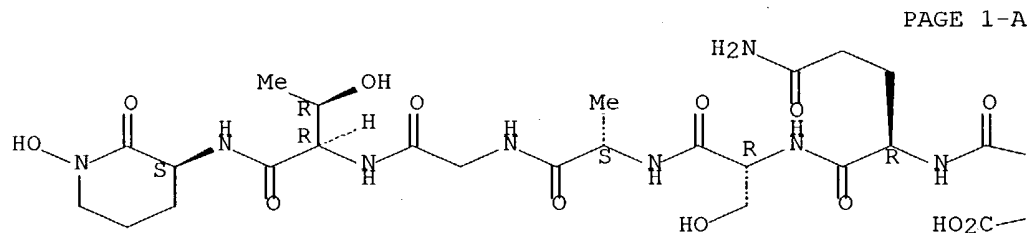
RN 235101-93-6 CAPLUS

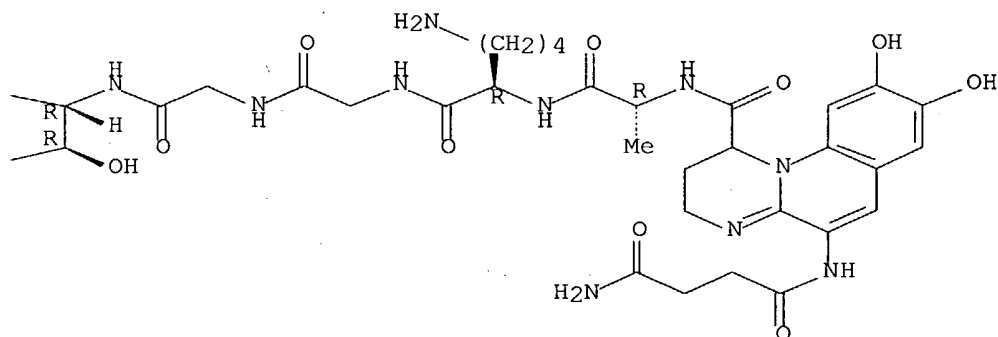
CN D-Allothreoninamide, N-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-D-lysylglycylglycyl-(3R)-3-hydroxy-D- α -aspartyl-D-glutaminy-D-seryl-L-alanylglycyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Currently available stereo shown.





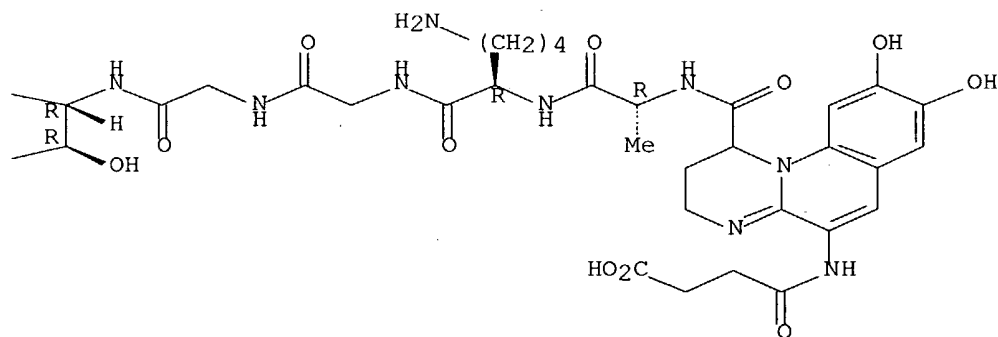
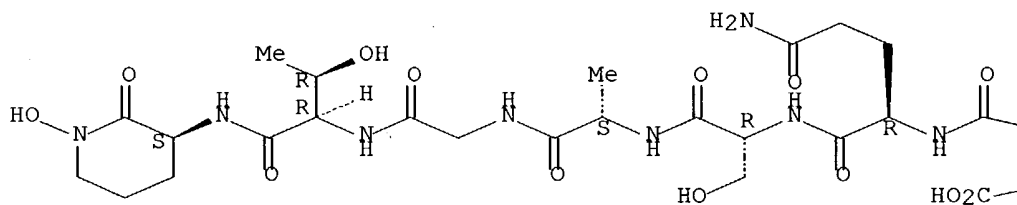
RN 235101-94-7 CAPLUS

CN D-Allothreoninamide, N-[[5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-D-lysylglycylglycyl-(3R)-3-hydroxy-D-α-aspartyl-D-glutaminy-D-seryl-L-alanyl-glycyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Currently available stereo shown.



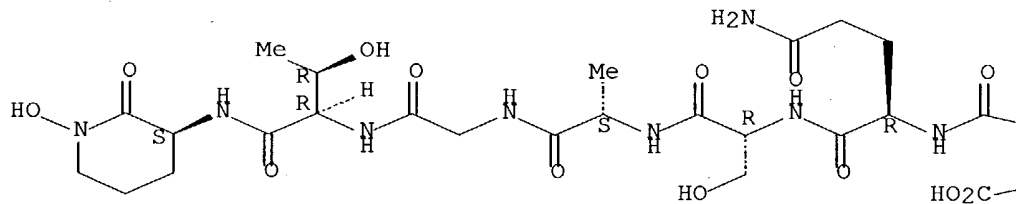
RE.CNT 7

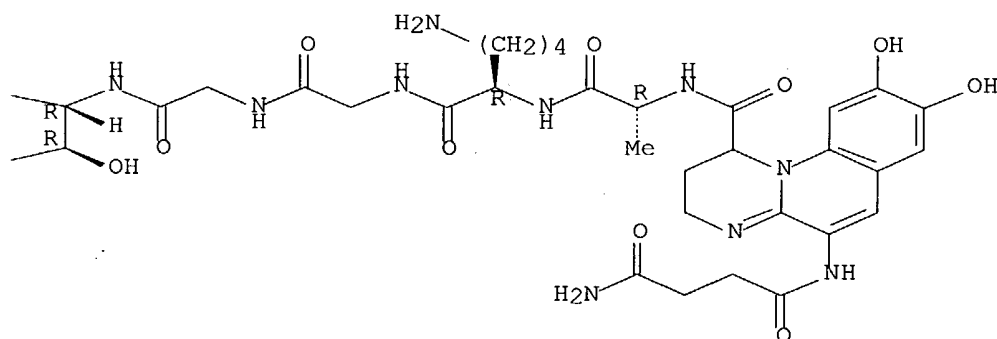
THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 20 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1999:334261 CAPLUS Full-text
 DN 131:141841
 TI Bacterial constituents. Part 80. A pyoverdin from the Antarctica strain 51W of *Pseudomonas fluorescens*
 AU Voss, Jessica; Taraz, Kambiz; Budzikiewicz, Herbert
 CS Institut Organische Chemie, Univ. Koln, Cologne, D-50939, Germany
 SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1999), 54(3/4), 156-162
 CODEN: ZNCBDA; ISSN: 0341-0382
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 AB From the strain 51W of *Pseudomonas fluorescens* living under extreme conditions at the Schirmacher Oasis (Antarctica) a pyoverdin was obtained. Its structure was elucidated by chemical degradation and spectroscopic methods. The NMR data of the pyoverdin and of its Ga(III) complex were compared. Appreciable influences of the metal on the chemical shifts of the atoms at its binding sites were observed. Thus, the structural elements involved in the complexation can be identified and coinciding signals of amino acids occurring more than once in the peptide chain can be separated.
 IT **235101-93-6**, Suca-Pyo51W **235101-94-7**, Suc-Pyo51W
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence) (a pyoverdin from the Antarctica strain 51W of *Pseudomonas fluorescens*)
 RN 235101-93-6 CAPLUS
 CN D-Allothreoninamide, N-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-D-lysylglycylglycyl-(3R)-3-hydroxy-D- α -aspartyl-D-glutaminyl-D-seryl-L-alanylglycyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Currently available stereo shown.

PAGE 1-A

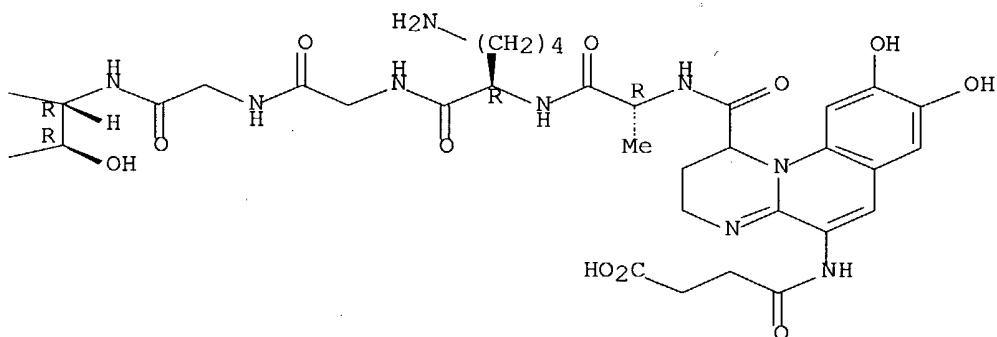
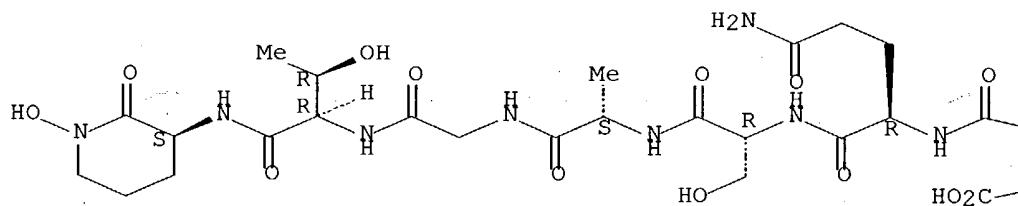




RN 235101-94-7 CAPLUS

CN D-Allothreoninamide, N-[[5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-D-lysylglycylglycyl-(3R)-3-hydroxy-D-α-aspartyl-D-glutaminyl-D-seryl-L-alanylglycyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Currently available stereo shown.



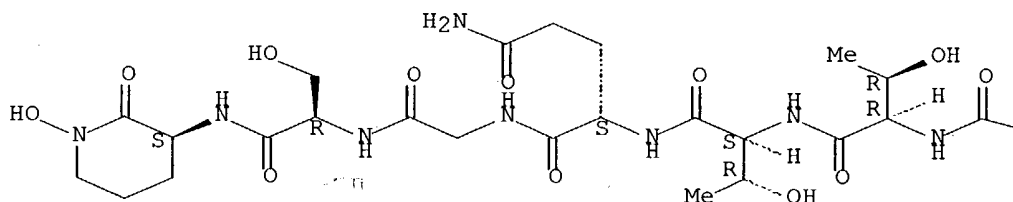
RE.CNT 7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

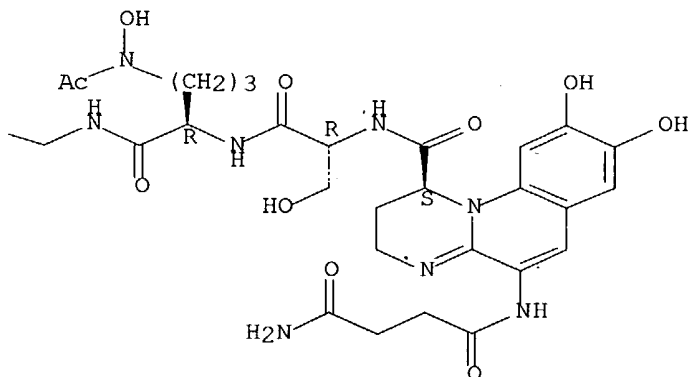
L14 ANSWER 21 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1999:157348 CAPLUS Full-text
 DN 130:279082
 TI Bacterial Constituents. Part 78. A new pyoverdin from *Pseudomonas aureofaciens*
 AU Beiderbeck, H.; Risse, D.; Budzikiewicz, H.; Taraz, K.
 CS Inst. Organische Chem., Univ. Koeln, Cologne, D-50939, Germany
 SO Zeitschrift fuer Naturforschung, C: Biosciences (1999), 54(1/2), 1-5
 CODEN: ZNCBDA; ISSN: 0341-0382
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 AB From *P. aureofaciens* a new pyoverdin was isolated and its structure was determined by spectroscopic methods and by partial degradation
 IT **222841-34-1DP**, Pyoverdin (*Pseudomonas aureofaciens*), iron complex
222841-35-2P, Pyoverdin (*Pseudomonas aureofaciens*)
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 PRP (Properties); PUR (Purification or recovery); BIOL (Biological study);
 OCCU (Occurrence); PREP (Preparation)
 (new pyoverdin from *Pseudomonas aureofaciens*)
 RN 222841-34-1 CAPLUS
 CN Pyoverdin (*Pseudomonas chlororaphis*) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

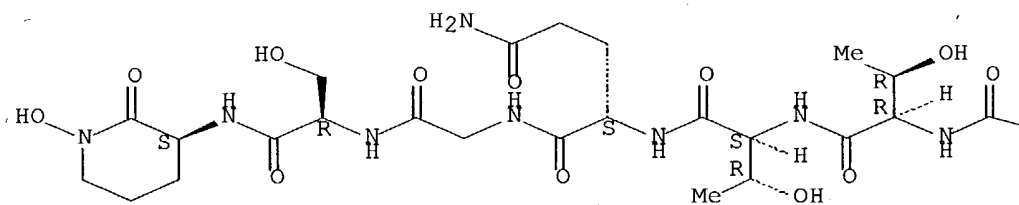


RN 222841-35-2 CAPLUS

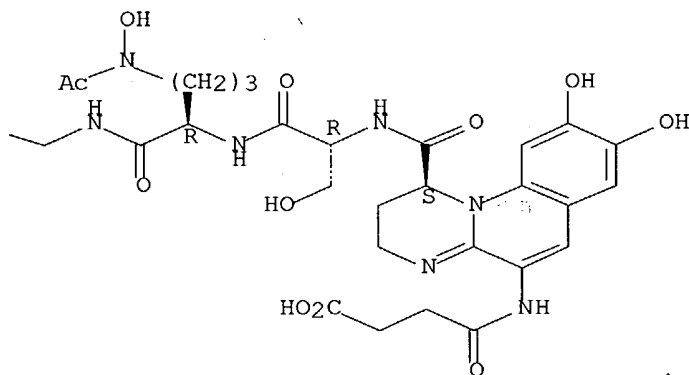
CN Pyoverdin (Pseudomonas chlororaphis), 1-[N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-serine]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 22 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:753582 CAPLUS Full-text

DN 130:121905

TI Siderotyping of fluorescent pseudomonads: characterization of pyoverdines

of *Pseudomonas fluorescens* and *Pseudomonas putida* strains from Antarctica

AU Meyer, Jean-Marie; Stintzi, Alain; Coulanges, Valerie; Shivaji, Sisinthy;

Voss, Jessica A.; Taraz, Kambiz; Budzikiewicz, Herbert

CS Laboratoire de Microbiologie et de Genetique, Universite Louis-Pasteur, UPRES A du CNRS no. 7010, Strasbourg, 67000, Fr.

SO Microbiology (Reading, United Kingdom) (1998), 144(11), 3119-3126
CODEN: MROBEO; ISSN: 1350-0872

PB Society for General Microbiology

DT Journal

LA English

AB Five independent fluorescent pseudomonad isolates originating from Antarctica were analyzed for their pyoverdine systems. A pyoverdine-related siderotyping, which involved pyoverdine-induced growth stimulation, pyoverdine-mediated iron uptake, pyoverdine anal. by electrophoresis and isoelec. focusing, revealed three different pyoverdine-related siderotypes among the five isolates. One siderotype, including *Pseudomonas fluorescens* 1W and *P. fluorescens* 10CW, was identical to that of *P. fluorescens* ATCC 13525. Two other strains, *P. fluorescens* 9AW and *Pseudomonas putida* 9BW, showed identical pyoverdine-related behavior to each other, whereas the fifth strain, *P. fluorescens* 51W, had unique features compared to the other strains or to a set of 12 fluorescent *Pseudomonas* strains used as comparison material. Elucidation of the structure of the pyoverdines produced by the Antarctic strains supported the accuracy of the siderotyping methodol. by confirming that pyoverdines from strains 1W and 10CW had the same structures as the *P. fluorescens* ATCC 13525 pyoverdine, whereas the 9AW and 9BW pyoverdines are probably identical with the pyoverdine of *P. fluorescens* strain 244. Pyoverdine from strain 51W appeared to be a novel pyoverdine since its structure was different from all previously established pyoverdine structures. Together with the conclusion that the Antarctic *Pseudomonas* strains have no special features at the level of their pyoverdines and pyoverdine-mediated iron metabolism compared to worldwide strains, the present work demonstrates that siderotyping provides a rapid means of screening for novel pyoverdines.

IT 219776-65-5, Pyoverdin (*Pseudomonas fluorescens* strain 9AW)

219776-66-6, Pyoverdin (*Pseudomonas fluorescens* strain 51W)

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

PRP (Properties); BIOL (Biological study); OCCU (Occurrence)

(siderotyping of fluorescent pseudomonads from Antarctica)

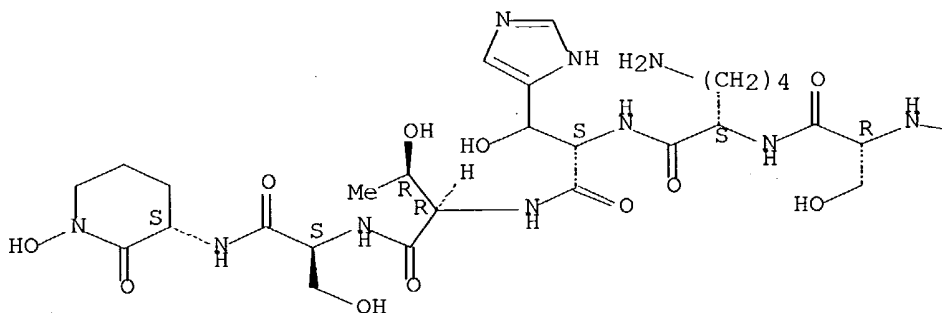
RN 219776-65-5 CAPLUS

CN L-Serinamide, N-[[[(1S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl- β -hydroxy-L-histidyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI)
(CA INDEX NAME)

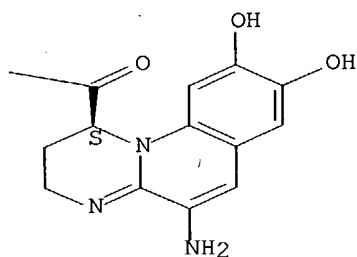
Absolute stereochemistry.

Currently available stereo shown.

PAGE 1-A



PAGE 1-B



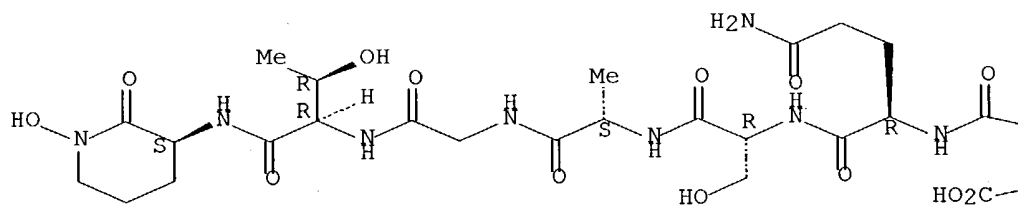
RN 219776-66-6 CAPLUS

CN D-Allothreoninamide, N-[[[(1S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-D-lysylglycylglycyl-3-hydroxy-D-α-aspartyl-D-glutaminy-D-seryl-L-alanylglycyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

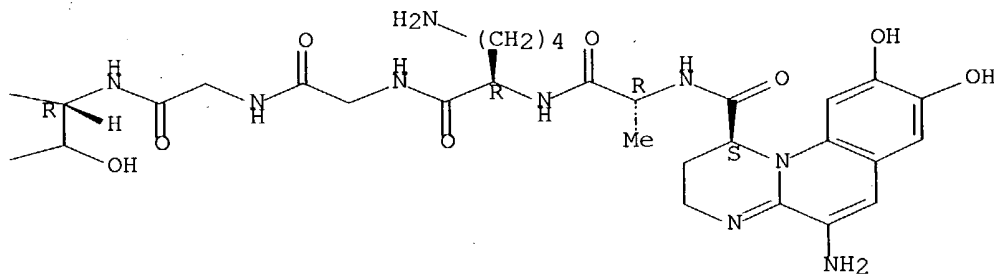
Absolute stereochemistry.

Currently available stereo shown.

PAGE 1-A



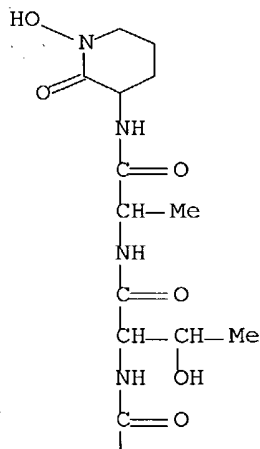
PAGE 1-B

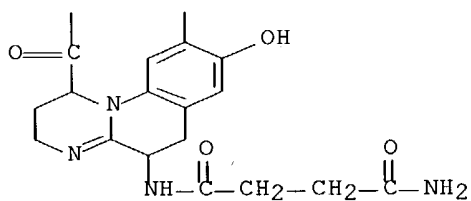
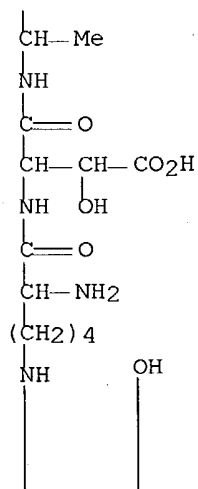


RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD

L14 ANSWER 23 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:709418 CAPLUS Full-text
 DN 130:78517
 TI Dihydropyoverdin-7-sulfonic acids. Unusual bacterial metabolites
 AU Budzikiewicz, H.; Fuchs, R.; Taraz, K.; Marek-Kozaczuk, M.; Skorupska, A.
 CS Inst. Organic Chem., Univ. Koeln, Cologne, D-50939, Germany
 SO Natural Product Letters (1998), 12(2), 125-130
 CODEN: NPLEEF; ISSN: 1057-5634
 PB Harwood Academic Publishers
 DT Journal
 LA English
 AB From the culture of Pseudomonas species 267 obtained from the
 rhizosphere of Triticum pseudobactin and pseudobactin A were isolated.
 These 2 compds. are the pyoverdins typical for Pseudomonas fluorescens,
 which establishes the identity of the strain. 2 Novel compds. were
 found in the cultural broth, viz. 2 7-sulfonic acid derivs. of
 pseudobactin A. Their structure elucidation and biogenetic implications
 will be presented.
 IT **79438-64-5**, Pseudobactin A **218432-99-6**
218433-00-2
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 BIOL (Biological study); OCCU (Occurrence)
 (dihydropyoverdin-7-sulfonic acids, pseudobactin and pseudobactin A
 metabolites from Pseudomonas 267)
 RN 79438-64-5 CAPLUS
 CN L-Alaninamide, N6-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3,5,6-
 tetrahydro-
 8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-
 piperidiny)- (9CI) (CA INDEX NAME)

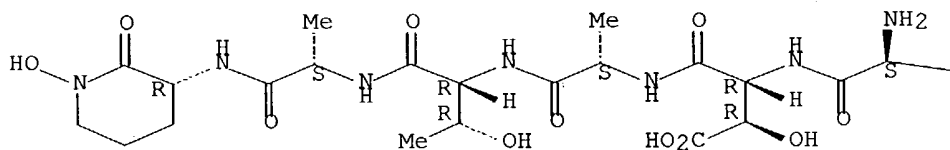
PAGE 1-A

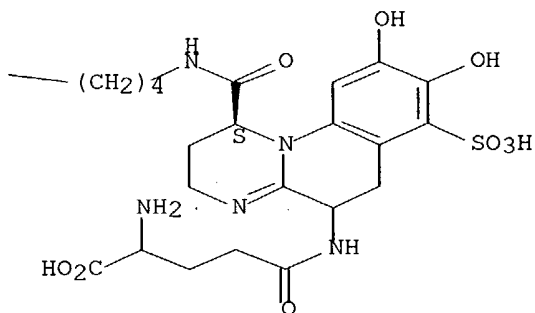




RN 218432-99-6 CAPLUS
 CN L-Alaninamide, N6-[γ-glutamyl-(1S)-5-amino-2,3,5,6-tetrahydro-8,9-dihydroxy-7-sulfo-1H-pyrimido[1,2-a]quinoline-1-carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



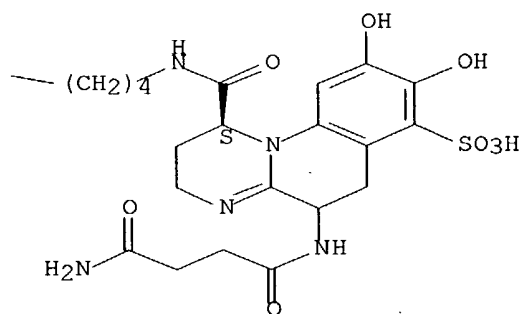
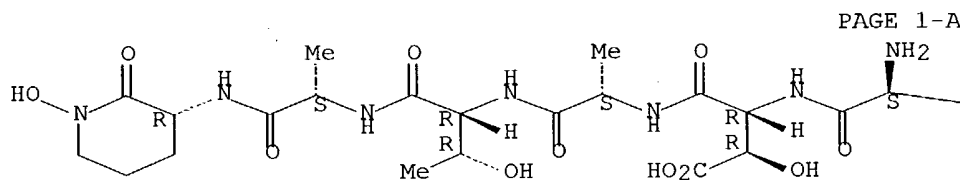


RN 218433-00-2 CAPLUS

CN L-Alaninamide, N6-[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3,5,6-tetrahydro-8,9-dihydroxy-7-sulfo-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-

L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 76975-04-7P, Pseudobactin 138145-39-8P
138145-41-2P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

PRP

(Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation).

(dihydropyoverdin-7-sulfonic acids, pseudobactin and pseudobactin A metabolites from Pseudomonas 267)

RN 76975-04-7 CAPLUS

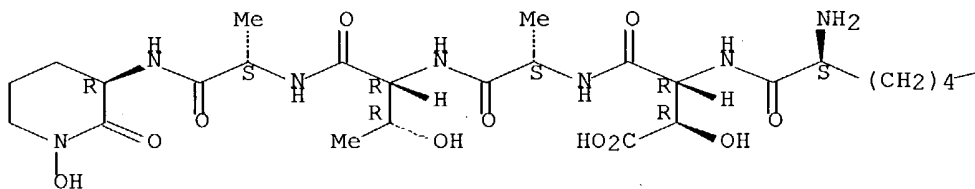
CN L-Alaninamide, N6-[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

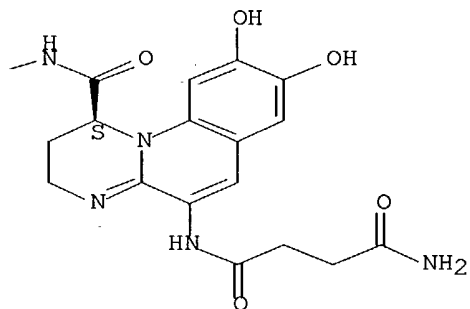
D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

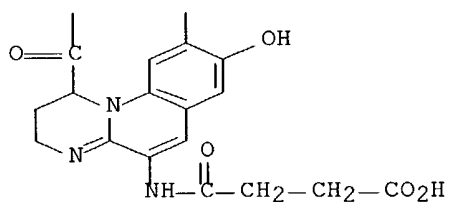
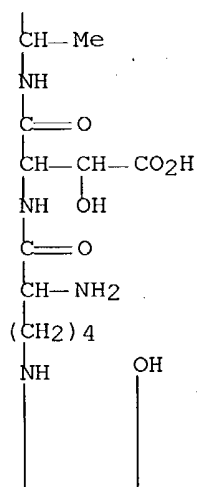
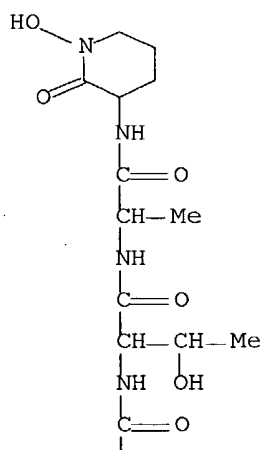


RN 138145-39-8 CAPLUS

CN L-Alaninamide, N6-[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3S)-3-hydroxy-

D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

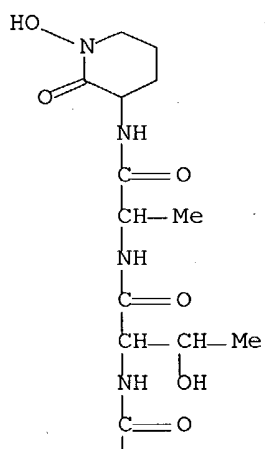


RN 138145-41-2 CAPLUS

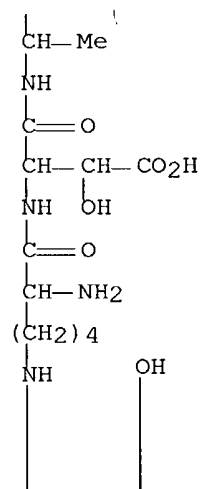
CN L-Alaninamide, N6-[[5-[(4-amino-4-carboxy-1-oxobutyl)amino]-2,3,5,6-tetrahydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-

(3S)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

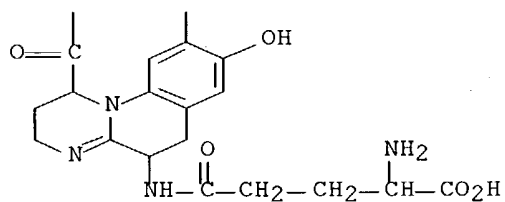
PAGE 1-A



PAGE 2-A



PAGE 3-A

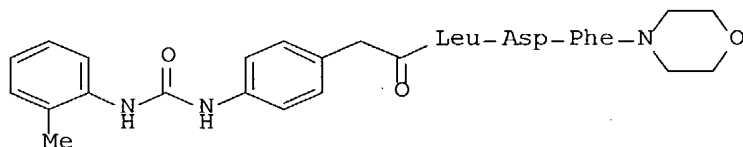
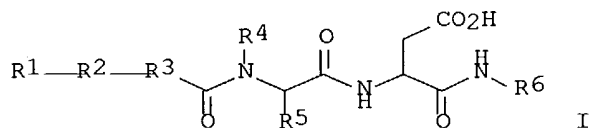


RE.CNT 12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 24 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:677800 CAPLUS Full-text
 DN 129:276355
 TI Preparation of peptides and peptidomimetics as VLA-4 antagonists
 IN He, Ya-Bo; Elices, Mariano J.; Arrhenius, Thomas S.
 PA Cytel Corporation, USA
 SO PCT Int. Appl., 153 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9842656	A1	19981001	WO 1998-US5709	19980320
	W: CA, JP				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT,				
SE					
PRAI	US 1997-821825		19970321		
OS	MARPAT 129:276355				
GI					

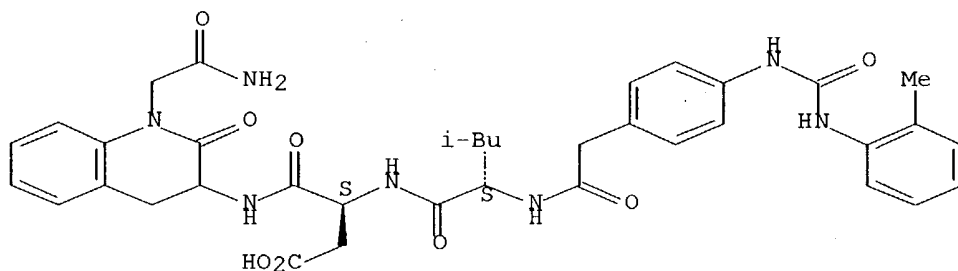


AB Title compds. I [R1 = alkyl, adamantyl, (un)substituted non-heterocyclic, heterocyclic, aromatic, or partially or fully saturated ring; R2 = lower alkyl, alkenyl, or alkynyl group in which each group optionally can contain a carbonyl, ether, thioether, aminocarbonyl group, etc., or E-C(R7)-F where R7 = S, O; E = CX1X2, NX3, or O; F = CX4X5, NX6, or O; X1-X6 = independently H or a lower alkyl, with the proviso that E and F are not simultaneously oxygen atoms and if R1 is an alkyl group, R2 must be of formula E-C(R7)-F; R3 = 5-, 6-, 6,5-, or 6,6-membered aromatic ring optionally containing 1-3 heteroatoms selected from the group O, N, S; R4 = H, lower alkyl; R5 = H, lower alkyl, (un)substituted lower alkyl amido group, or a 5- or 6- membered non-heterocyclic saturated ring connected directly by a bond or through a lower alkyl group; R6 = substituted azepine, or CH(R8)COAR9R10 where A = N, O; R8 = H, lower alkyl, hydroxyalkyl, thioalkyl, a ring structure connected directly by a bond or through a lower alkyl group, or R8 and R9 together form a ring structure, etc.; R9 = lower alkyl, hydroxyalkyl, morpholino group, or together with R10 form a ring structure; R10 = (un)substituted lower alkyl, or together with R9 form a ring structure; when A = O, R10 is absent] and pharmaceutically- acceptable derivs. thereof. were prepared as VLA-4 antagonists. Thus, II (solution phase preparation given) was assayed for binding inhibition potency (IC50 = 0.4 nM) toward Jurkat cells.

IT 213989-58-3P

RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides and peptidomimetics as VLA-4 antagonists)
RN 213989-58-3 CAPLUS
CN L- α -Asparagine, N-[[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl
]acetyl]-L-leucyl-N-[1-(2-amino-2-oxoethyl)-1,2,3,4-tetrahydro-2-oxo-3-
quinolinyl]- (9CI) (CA INDEX NAME)

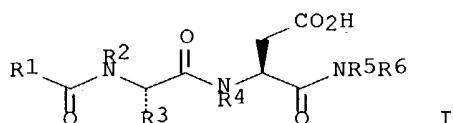
Absolute stereochemistry.



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 25 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:668012 CAPLUS Full-text
 DN 129:290438
 TI Preparation of CS-1 peptidomimetics and their compositions
 IN Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.
 PA Cytel Corp., USA
 SO U.S., 81 pp., Cont.-in-part of U.S. Ser. No. 349,024.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5821231	A	19981013	US 1995-461056	19950605
	CA 2177840	AA	19950615	CA 1994-2177840	19941205
	CN 1142832	A	19970212	CN 1994-194969	19941205
	US 5688913	A	19971118	US 1995-435286	19950505
	US 6117840	A	20000912	US 1997-837154	19970414
	US 6103870	A	20000815	US 1997-923026	19970903
PRAI	US 1993-164101	B2	19931206		
	US 1994-349024	A2	19941202		
	US 1995-435286	A1	19950505		
OS	MARPAT 129:290438				
GI					



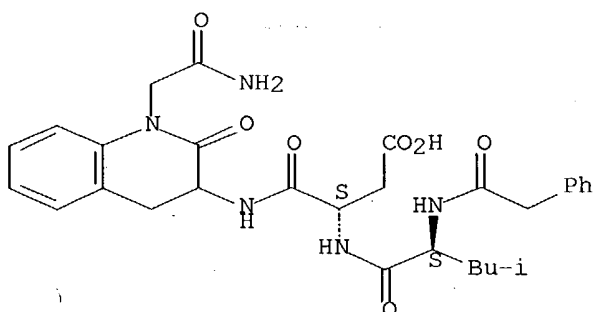
AB Peptidomimetics I (R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, Me or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, 1,1-diphenylmethine, or the R5 ring structure) were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

IT **209601-18-3P 209601-35-4P 209601-64-9P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of CS-1 peptidomimetics and their comps.)

RN 209601-18-3 CAPLUS

CN L-α-Asparagine, N-(phenylacetyl)-L-leucyl-N-[1-(2-amino-2-oxoethyl)-1,2,3,4-tetrahydro-2-oxo-3-quinoliny]- (9CI) (CA INDEX NAME)

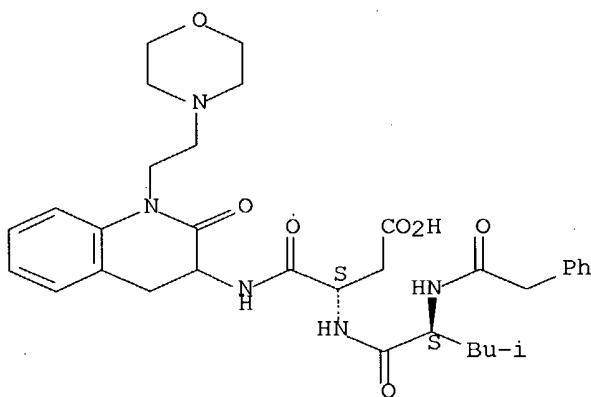
Absolute stereochemistry.



RN 209601-35-4 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-[2-(4-morpholinyl)ethyl]-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

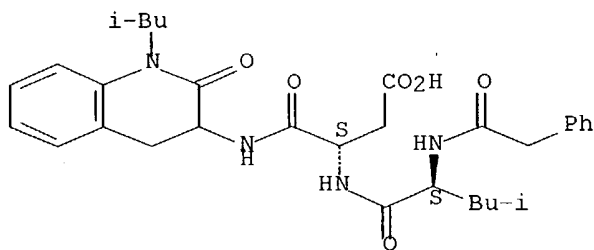
Absolute stereochemistry.



RN 209601-64-9 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-(2-methylpropyl)-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

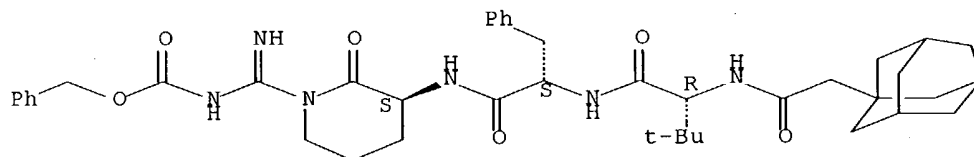
Absolute stereochemistry.



RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 26 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:484456 CAPLUS Full-text
 DN 129:213364
 TI Peptide aldehyde inhibitors of the kallikreins: an investigation of
 subsite interactions with tripeptides containing structural variations
 at the amino terminus
 AU Garrett, G. S.; Correa, P. E.; Mcphail, S. J.; Tornheim, K.; Burton, J.
 A.; Eickhoff, D. J.; Engerholm, G. G.; Mciver, J. M.
 CS Corporate Research Division, Procter and Gamble Company, Miami Valley
 Laboratories, Cincinnati, OH, 45253-8707, USA
 SO Journal of Peptide Research (1998), 52(1), 60-71
 CODEN: JPERFA; ISSN: 1397-002X
 PB Munksgaard International Publishers Ltd.
 DT Journal
 LA English
 AB A series of tripeptide aldehyde derivs. containing variations at the P3
 subsite and the amino terminus has been prepared and evaluated for
 trypsin-like serine protease inhibition. These compds. exhibit strong
 in vitro inhibition of human plasma kallikrein (HPK), porcine pancreatic
 kallikrein (PPK) and human plasmin (HP). As suspected from an
 examination of a related crystal structure, the presence of a
 hydrophobic residue (adamantyl) at the amino terminus dramatically
 improves the binding to PPK. The adamantyl group, however, represents a
 peak in binding; larger residues cause the binding to be reduced, and
 thus are less well accommodated in this subsite. Although both HP and
 HPK also can accept large mol. volume at the amino terminus, they do not
 exhibit the same preference for large residues at this subsite that is
 demonstrated by PPK. Selectivity differences also are observed with P3
 subsite substitution; with PPK preferring a bulky, but compact side-
 chain (t-butyl) and HP and HPK preferring a more extended (e.g. benzyl)
 group.
 IT **150906-26-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT(Reactant or reagent)(synthesis of peptide aldehyde inhibitors of
 kallikreins)
 RN 150906-26-6 CAPLUS
 CN L-Phenylalaninamide, 3-methyl-N-(tricyclo[3.3.1.1^{3,7}]dec-1-ylacetyl)-D-
 valyl-N-[(3S)-1-[imino[[(phenylmethoxy)carbonyl]amino]methyl]-2-oxo-3-
 piperidiny]- (9CI) (CA INDEX NAME)

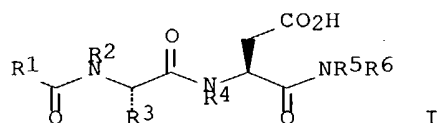
Absolute stereochemistry.



RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 27 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:427769 CAPLUS Full-text
 DN 129:95722
 TI Preparation of CS-1 peptidomimetics and their compositions
 IN Arrhenius, Thomas S.; Elices, Mariano J.; Gaeta, Federico C. A.
 PA Cytel Corp., USA
 SO U.S., 80 pp., Cont.-in-part of U.S. Ser. No. 349,024.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5770573	A	19980623	US 1995-462219	19950605
	CA 2177840	AA	19950615	CA 1994-2177840	19941205
	CN 1142832	A	19970212	CN 1994-194969	19941205
	US 5688913	A	19971118	US 1995-435286	19950505
	US 6117840	A	20000912	US 1997-837154	19970414
	US 6103870	A	20000815	US 1997-923026	19970903
PRAI	US 1993-164101	B2	19931206		
	US 1994-349024	A2	19941202		
	US 1995-435286	A1	19950505		
OS	MARPAT 129:95722				
GI					



AB Peptidomimetics I (R1 = alkyl, aminoalkyl, or a ring structure which may form at R1, between R1 and R2 or between R1 and R4; R2 = H, Me or R2 and R1 form the R1 ring structure group; R3 = alkyl, alkyl alc., thioalkyl or a ring structure; R4 = H or R4 and R1 form the R1 ring structure; R5 = H or R5 and R6 form a ring structure; R6 = benzyl, 1,1-diphenylmethine, or the R5 ring structure) were prepared as inhibitors of the binding between the VLA-4 receptor and the fibronectin CS-1 domain. Thus, N-phenylacetyl-Leu-Asp-Phe-D-Pro-NH2 was prepared and assayed for binding inhibition potency (313 relative to a standard compound).

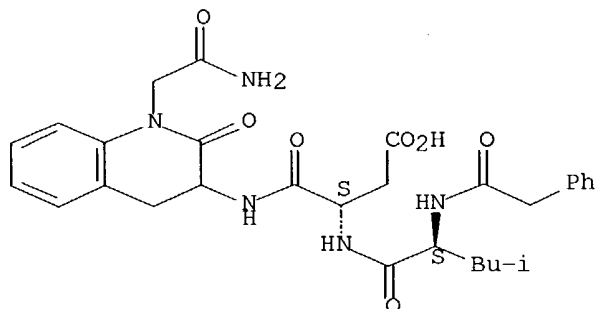
IT 209601-18-3P 209601-35-4P 209601-64-9P

RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic
 use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of CS-1 peptidomimetics and their comps.)

RN 209601-18-3 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1-(2-amino-2-oxoethyl)-
 1,2,3,4-tetrahydro-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

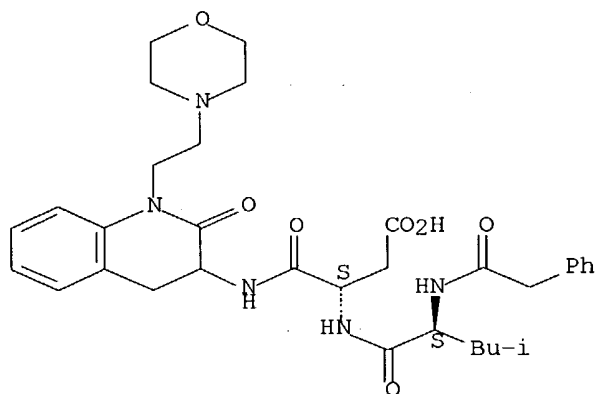
Absolute stereochemistry.



RN 209601-35-4 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-[2-(4-morpholinyl)ethyl]-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

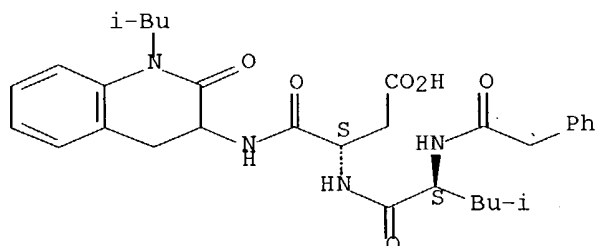
Absolute stereochemistry.



RN 209601-64-9 CAPLUS

CN L- α -Asparagine, N-(phenylacetyl)-L-leucyl-N-[1,2,3,4-tetrahydro-1-(2-methylpropyl)-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

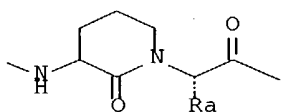
Absolute stereochemistry.



RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 28 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:405973 CAPLUS Full-text
 DN 129:81966
 TI Inhibitors of peptide binding to MHC class II proteins
 IN Luke, Richard William Arthur; Cotton, Ronald
 PA Zeneca Ltd., UK; Luke, Richard William Arthur; Cotton, Ronald
 SO PCT Int. Appl., 44 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9825951	A1	19980618	WO 1997-GB3397	19971209
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9854047	A1	19980703	AU 1998-54047	19971209
	EP 946589	A1	19991006	EP 1997-947807	19971209
	EP 946589	B1	20031001		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2001505905	T2	20010508	JP 1998-526363	19971209
	AT 251178	E	20031015	AT 1997-947807	19971209
	US 6184207	B1	20010206	US 1999-319870	19990614
PRAI	GB 1996-25865	A	19961212		
	WO 1997-GB3397	W	19971209		
OS	MARPAT 129:81966				
GI					



I

AB Peptides P-AA1-AA2-AA3-AA4-AA5-AA6-AA7-AA8-Q [AA3 together with AA4 or AA4 together with AA5 or AA6 together with AA7 form a group of formula I in which Ra is H (II) or alkyl; the remainder of AA1, AA2, AA3, AA4, AA5, AA6, AA7, and AA8 are L-amino acid residues; P is a hydrophobic residue; Q is OH, NH2, NRcRd (Rc is alkyl, 2-carbamoylcyclopentyl, 2-pyridylmethyl, 4-carbamoylcyclohexyl, 4-carbamoylcyclohexylmethyl, 3- or 4-carbamoylphenyl, etc. and Rd is H or alkyl), (un)substituted 1-piperazinyl, or 1-piperidyl] were prepared as inhibitors of peptide binding to MHC class II proteins. Thus, Phv-Arg-Ala-Ala-Ala-Thr-II-Ala-Papa-NH2 [Phv = 5-phenylvaleryl, Papa = 4-aminophenylacetic acid residue] was prepared by the solid-phase method.

IT **209163-22-4P 209163-23-5P 209163-24-6P**
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (inhibitors of peptide binding to MHC class II proteins)

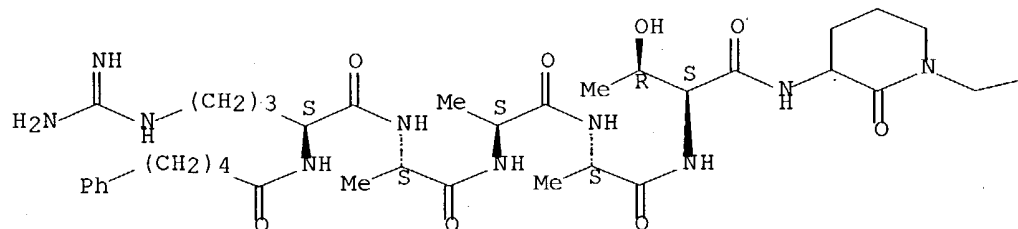
RN 209163-22-4 CAPLUS

CN L-Alaninamide, N2-(1-oxo-5-phenylpentyl)-L-arginyl-L-alanyl-L-alanyl-L-

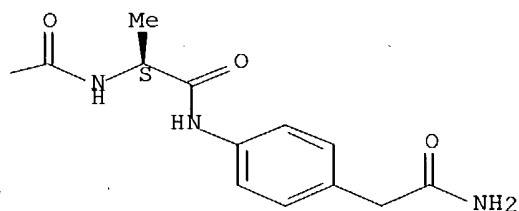
alanyl-L-threonyl-3-amino-2-oxo-1-piperidineacetyl-N-[4-(2-amino-2-oxoethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

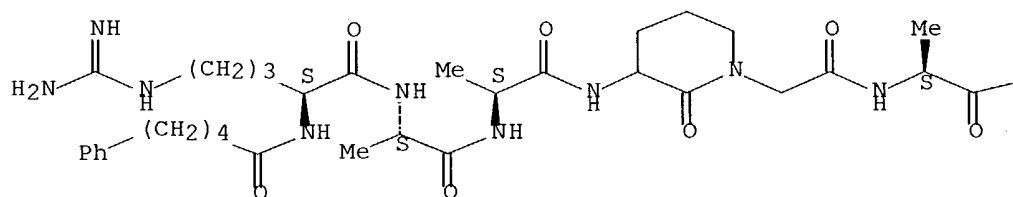


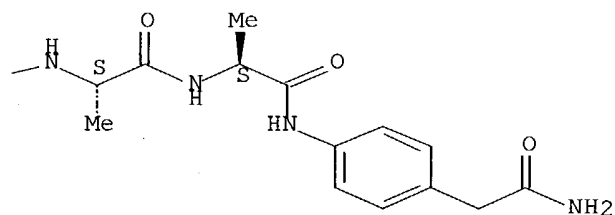
RN 209163-23-5 CAPLUS

CN L-Alaninamide, N2-(1-oxo-5-phenylpentyl)-L-arginyl-L-alanyl-L-alanyl-3-amino-2-oxo-1-piperidineacetyl-L-alanyl-L-alanyl-N-[4-(2-amino-2-oxoethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

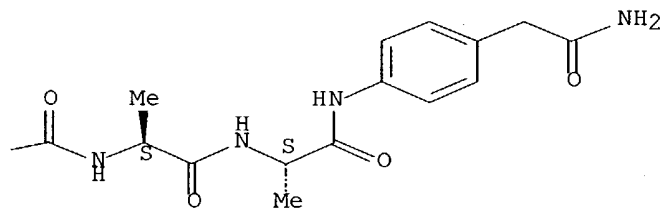
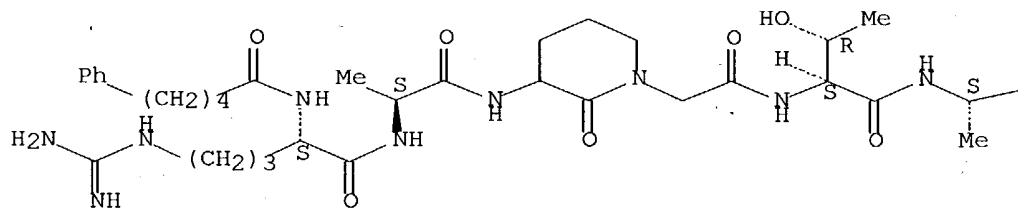
PAGE 1-A





RN 209163-24-6 CAPLUS
 CN L-Alaninamide, N2-(1-oxo-5-phenylpentyl)-L-arginyl-L-alanyl-3-amino-2-oxo-
 1-piperidineacetyl-L-threonyl-L-alanyl-L-alanyl-N-[4-(2-amino-2-oxoethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 29 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:348905 CAPLUS Full-text

DN 129:81948

TI The synthesis and antibacterial activity of two pyoverdinin-ampicillin conjugates, entering *Pseudomonas aeruginosa* via the pyoverdinin-mediated iron uptake pathway

AU Kinzel, Olaf; Tappe, Robert; Gerus, Igor; Budzikiewicz, Herbert

CS Institute for Organic Chemistry, Koln, D-50939, Germany

SO Journal of Antibiotics (1998), 51(5), 499-507

CODEN: JANTAJ; ISSN: 0021-8820

PB Japan Antibiotics Research Association

DT Journal

LA English

AB Two pyoverdinin-ampicillin conjugates were synthesized and their structures were confirmed by mass spectrometry and NMR spectroscopy. In contrast to ampicillin, the conjugates exhibited high antibacterial activity against *Pseudomonas aeruginosa* ATCC 15692 and ATCC 27853, effective only against the strain which is using the parent pyoverdinin for iron uptake. This suggests that the conjugates enter the bacterial cell via the ferripyoverdinin uptake pathway. Growth stimulation studies with conjugates hydrolyzed at the β -lactam ring of the ampicillin moiety supported this view.

IT **209345-69-7P**

RL: BAC (Biological activity or effector, except adverse); BPR

(Biological

process); BSU (Biological study, unclassified); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation); PROC

(Process)

(preparation and antibacterial activity of pyoverdinin-ampicillin conjugates

entering *Pseudomonas aeruginosa* via the pyoverdinin-mediated iron uptake pathway)

RN 209345-69-7. CAPLUS

CN L-Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-N5-formyl-

N5-

hydroxy-D-ornithyl-N5-[10-[[[(1R)-2-[[[(2S,5R,6R)-2-carboxy-3,3-dimethyl-

7-

oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]amino]-2-oxo-1-

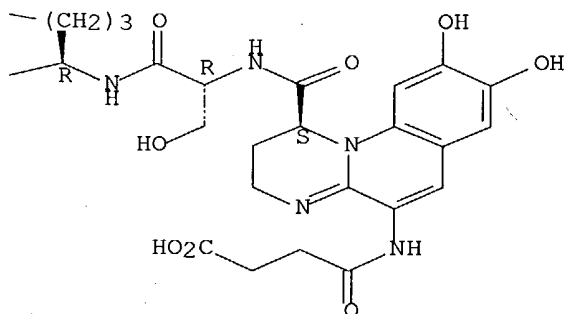
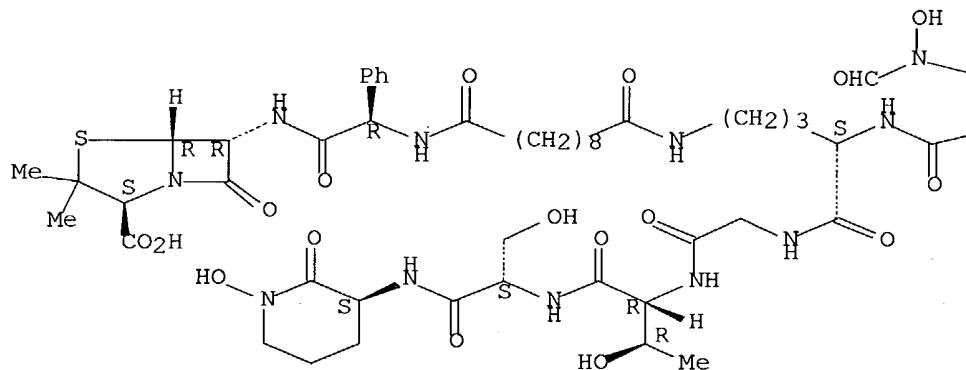
phenylethyl]amino]-

1,10-dioxodecyl]-L-ornithylglycyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-

oxo-3-

piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 148337-19-3 148337-19-3D, iron(III) conjugate

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and antibacterial activity of pyoverdine-ampicillin conjugates

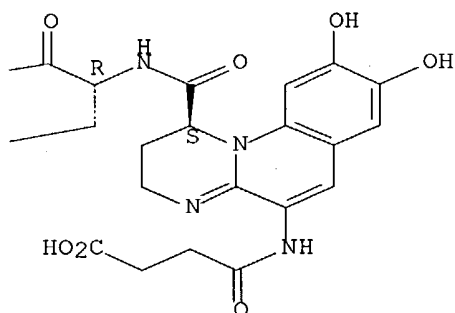
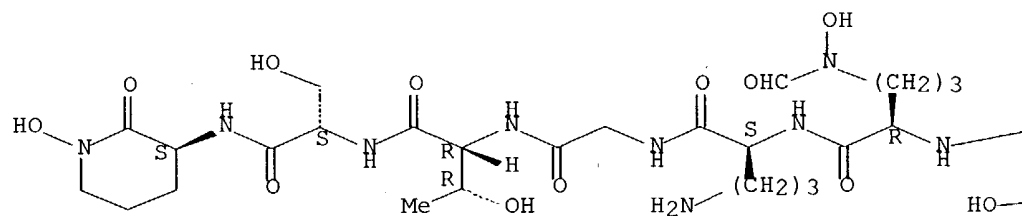
entering *Pseudomonas aeruginosa* via the pyoverdine-mediated iron uptake pathway)

RN 148337-19-3 CAPLUS

CN L-Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-N5-formyl-

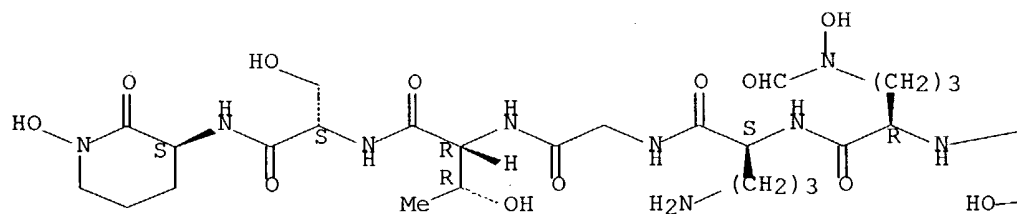
N5-hydroxy-D-ornithyl-L-ornithylglycyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

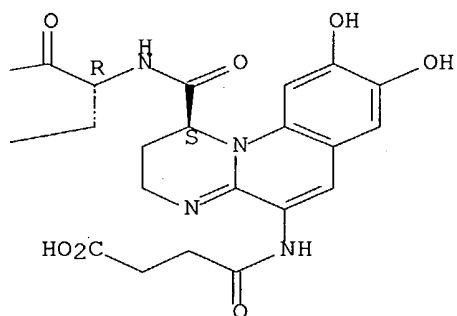
Absolute stereochemistry.



RN 148337-19-3 CAPLUS
 CN L-Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-N5-formyl-
 N5-hydroxy-D-ornithyl-L-ornithylglycyl-D-allo-threonyl-N-[(3S)-1-hydroxy-2-oxo-
 3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





IT 209345-69-7DP, iron(III) conjugate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation and antibacterial activity of pyoverdin-ampicillin conjugates

entering *Pseudomonas aeruginosa* via the pyoverdin-mediated iron uptake

pathway)

RN 209345-69-7 CAPLUS

CN L-Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-N5-formyl-

N5-

hydroxy-D-ornithyl-N5-[10-[[[(1R)-2-[[[(2S,5R,6R)-2-carboxy-3,3-dimethyl-

7-

oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]amino]-2-oxo-1-

phenylethyl]amino]-

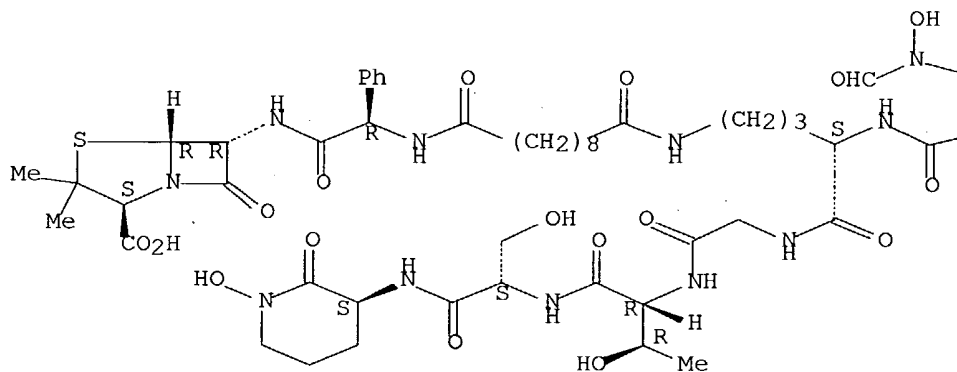
1,10-dioxodecyl]-L-ornithylglycyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-

oxo-3-

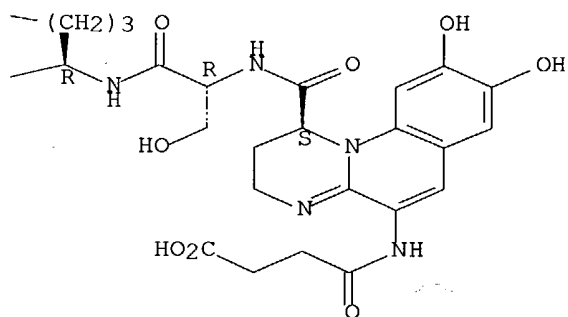
piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 30 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:146693 CAPLUS Full-text
 DN 128:205143
 TI Preparation of peptidyl inhibitors of factor Xa
 IN Marlowe, Charles K.; Scarborough, Robert M.; Laibelman, Alan M.; Sinha, Uma; Zhu, Bing-yan
 PA COR Therapeutics, Inc., USA
 SO U.S., 25 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 5721214	A	19980224	US 1995-485433	19950607
PRAI	US 1995-485433		19950607		
OS	MARPAT 128:205143				

AB Novel compds. ZQ(CH₂)_mCHR₄(GWR₅)C(:E)DR₃CR₂R₆C(:J)NR₁CHY(CH₂)_nAX [m, n = 0-4; Y = CHO, COCF₃, COCF₂CF₃, etc.; A = absent, piperidinyl, pyrrolidinyl, cyclopropyl, Ph, etc.; R₁, R₂, R₃ = H, alkyl; R₄ = H, Me; J, E = O, H₂; D = N, CH, NCH₂, NCH₂CH₂, CHCH₂; Q = absent, piperidinyl, pyrrolidinyl, cycloalkyl, Ph, naphthyl, pyridyl, etc.; G = N, CH, H; R₅ = H, alkyl, or absent; R₆ = H, Me; W = absent, H, arylacetyl, heteroarylacetyl, arylsulfonyl, alkylaminocarbonyl, etc.; X, Z = NR'R'', NHC(NR'R'') : NH, NHC(NHR') : NR'', SC(NR'R'') : NH, etc. (R' and R'' are H, alkyl, arylalkyl, aryl or R'R'' is alkylene)] or their salts were prepared as factor Xa inhibitors. Thus, Boc-D-Arg-Gly-Arg-H (Boc = tert-butoxycarbonyl) was prepared by reduction-hydrogenolysis of Boc-D-Arg(Cbz₂)-Gly-Arg(N-Cbz)-lactam (Cbz = benzyloxycarbonyl), which was prepared by peptide coupling in solution. The product was evaluated in rabbits for biol. half-life, antithrombotic efficacy, and effects on hemostasis and hematol. parameters.

IT **186369-07-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

(preparation of peptidyl inhibitors of factor Xa)

RN 186369-07-3 CAPLUS

CN Glycinamide; N₂-[1,4-dioxo-4-(phenylmethoxy)butyl]-N₅-

[imino[(phenylmethoxy)carbonyl]amino]methyl]-N₅-

[(phenylmethoxy)carbonyl]-

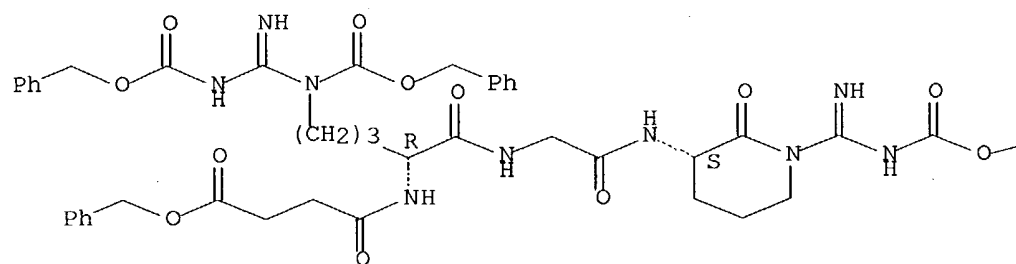
D-ornithyl-N-[(3S)-1-[imino[(phenylmethoxy)carbonyl]amino]methyl]-2-

oxo-3-

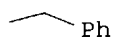
piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

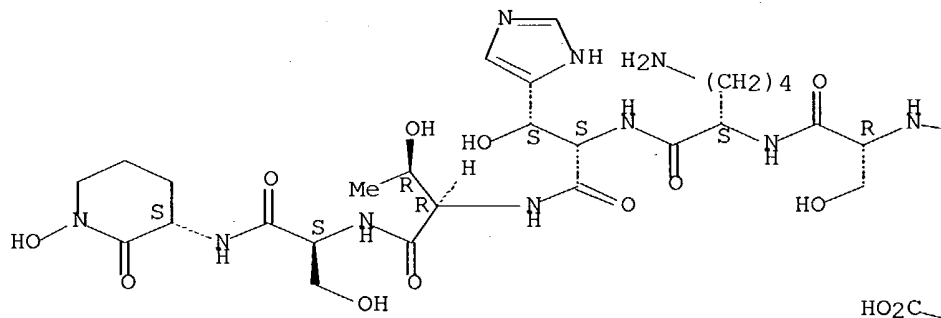


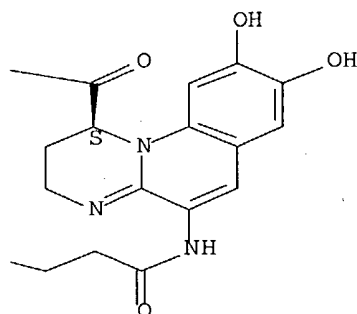
RE.CNT 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 31 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1998:68911 CAPLUS Full-text
 DN 128:177974
 TI Identical pyoverdines from *Pseudomonas fluorescens* 9AW and from
Pseudomonas putida 9BW
 AU Budzikiewicz, Herbert; Kilz, S.; Taraz, K.; Meyer, J. M.
 CS Institut Organische Chemie, Universitaet Koeln, Cologne, D-50939,
 Germany
 SO Zeitschrift fuer Naturforschung, C: Biosciences (1997), 52(11/12), 721-
 728
 CODEN: ZNCBDA; ISSN: 0341-0382
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 AB From *P. fluorescens* 9AW and from *P. putida* 9BW identical pyoverdine-type
 siderophores were isolated and their structures were elucidated by
 spectroscopy and degradation studies. These novel compds. are of
 interest as they contain L-threo- β -hydroxy His in their peptide chains,
 an amino acid so far encountered in nature only rarely. The co-
 occurrence of the same pyoverdine in different *Pseudomonas* species and
 its significance for the classification is discussed.
 IT **203261-53-4P**
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 PRP
 (Properties); PUR (Purification or recovery); RCT (Reactant); SPN
 (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence);
 PREP
 (Preparation); RACT (Reactant or reagent)
 (pyoverdines from *Pseudomonas fluorescens* and *P. putida*)
 RN 203261-53-4 CAPLUS
 CN L-Serinamide, N-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-
 (β S)- β -hydroxy-L-histidyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-
 3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





IT 203261-55-6P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

PRP

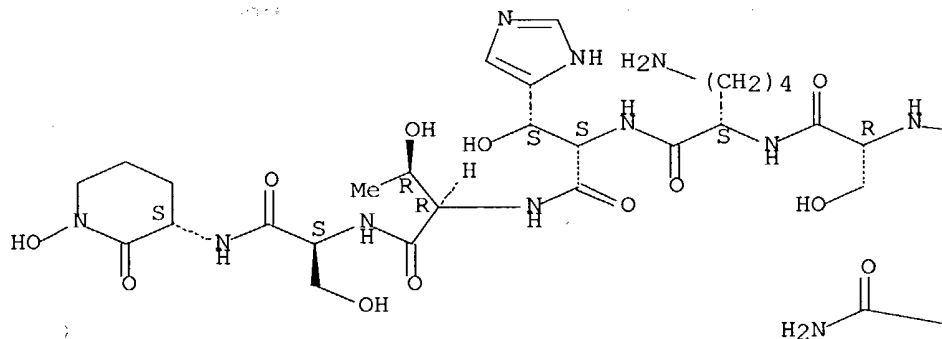
(Properties); PUR (Purification or recovery); SPN (Synthetic preparation);

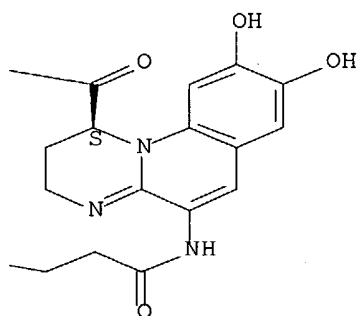
BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(pyoverdines from *Pseudomonas fluorescens* and *P. putida*)

RN 203261-55-6 CAPLUS

CN L-Serinamide, N-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-(βS)-β-hydroxy-L-histidyl-D-allothreonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

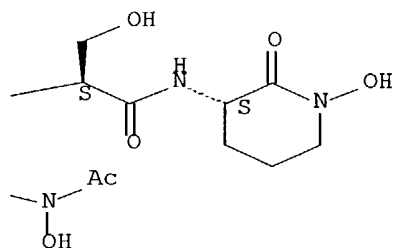
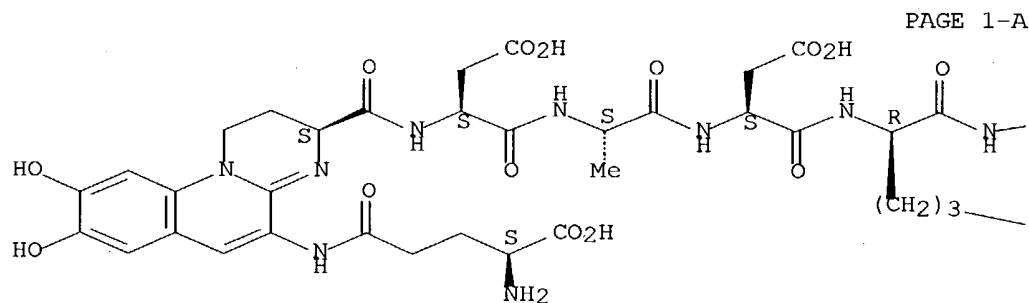
Absolute stereochemistry.





L14 ANSWER 32 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:590720 CAPLUS Full-text
 DN 127:275116
 TI Absolute configuration of the isopyoverdin chromophore
 AU Michalke, R.; Taraz, K.; Budzikiewicz, H.; Thonart, P.; Jacques, P.
 CS Institut Organische Chemie, Universitat Koln, Cologne, D-50939, Germany
 SO Zeitschrift fuer Naturforschung, C: Biosciences (1997), 52(7/8), 549-550
 CODEN: ZNCBDA; ISSN: 0341-0382
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 AB By ozonolytic degradation of the chromophore of isopyoverdin from *Pseudomonas putida* BTP 1 L-2,4-diaminobutyric acid was obtained. This proves that the C-3 of the chromophore is S-configured.
 IT **159325-01-6**, Isopyoverdin
 RL: PRP (Properties)
 (isopyoverdin chromophore configuration of *Pseudomonas putida*)
 RN 159325-01-6 CAPLUS
 CN L-Serinamide, L- γ -glutamyl-(3S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinoline-3-carbonyl-L- α -aspartyl-L-alanyl-L- α -aspartyl-N5-acetyl-N5-hydroxy-D-ornithyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 33 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1997:362837 CAPLUS Full-text

DN 127:91020

TI Surface signaling: novel transcription initiation mechanism starting from the cell surface

AU Braun, Volkmar

CS Mikrobiologie/Membranphysiologie, Universitat Tübingen, Tübingen, D-72076, Germany

SO Archives of Microbiology (1997), 167(6), 325-331
CODEN: AMICCW; ISSN: 0302-8933

PB Springer

DT Journal; General Review

LA English

AB A review with 36 refs. Transcription of the ferric citrate transport genes of *Escherichia coli* is induced by a novel mechanism. Ferric citrate, the inducer, does not have to enter the cytoplasm to initiate transcription. Interaction of ferric citrate with the outer membrane receptor protein FecA induces transcription of the fec transport gene operon consisting of the fecIRABCDE genes. A signal from FecA occupied with ferric citrate is transmitted across the outer membrane into the periplasm with the help of the electrochem. potential of the cytoplasmic membrane and the Ton system. The signal is then transduced across the cytoplasmic membrane by the FecR protein, which in turn activates the FecI σ -factor that directs the RNA polymerase core-enzyme to the fec transport gene promoter. The promoter of the regulatory genes fecI and fecR is not controlled by ferric citrate but is regulated by iron via the Fur repressor. It is proposed that the information flux from the cell surface to the cytoplasm involves a series of conformational changes of the proteins FecA, FecR, and FecI in that order. The level of the regulatory proteins FecI and FecR is adjusted to the intracellular iron concentration and det. the degree of the response of the cell to ferric citrate in the medium. Ferric citrate induces transcription of the fec transport genes under iron-limiting conditions. A regulatory advice similar to the ferric citrate transport system exists in *Pseudomonas putida* WCS358. The synthesis of the outer membrane receptor PupB, involved in the transport of the ferric pseudobactins BN7 and BN8, is induced by the ferric siderophores and requires PupB and two proteins homologous to FecI and FecR.

IT 76975-04-7D, Pseudobactin, iron complexes

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)

(inducer; transcription of the ferric pseudobactins transport genes

is

induced by a novel mechanism starting from the cell surface)

RN 76975-04-7 CAPLUS

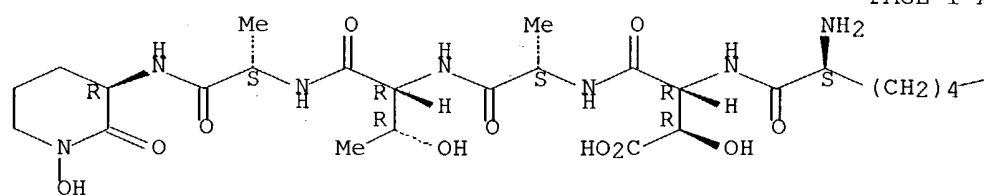
CN L-Alaninamide, N6-[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

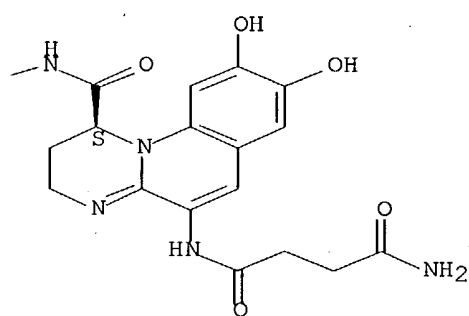
D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 34 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:121403 CAPLUS Full-text
 DN 126:131783
 TI Preparation of peptides as inhibitors of factor Xa
 IN Marlowe, Charles K.; Scarborough, Robert M.; Laibelman, Alan M.; Sinha, Uma; Zhu, Bing-yan
 PA Cor Therapeutics, Inc., USA
 SO PCT Int. Appl., 76 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9640743	A2	19961219	WO 1996-US9285	19960605
	WO 9640743	A3	19970123		
	W:		AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG		
	RW:		KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN		
	US 5919765	A	19990706	US 1995-483470	19950607
	CA 2224076	AA	19961219	CA 1996-2224076	19960605
	AU 9665902	A1	19961230	AU 1996-65902	19960605
	AU 710408	B2	19990923		
	EP 846125	A2	19980610	EP 1996-925254	19960605
	R:		AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI		
	JP 11507626	T2	19990706	JP 1996-501639	19960605
	ZA 9604753	A	19970227	ZA 1996-4753	19960606
	US 6245743	B1	20010612	US 1998-77001	19980515
PRAI	US 1995-483470	A	19950607		
	WO 1996-US9285	W	19960605		

OS MARPAT 126:131783

AB Peptides

R1(CH2)pX1(CH2)mCR2(X2R3R4)C(:Y1)X3R5CR6R7C(:Y2)NR8CHR9(CH2)nX4(C H2)qR10 (X1 = piperidinyl, pyrrolidinyl, cycloalkyl, Ph, substituted Ph, naphthyl, pyridyl, or null; X2 = N, CH, H; X3 = N, CH, NCH2, NCH2CH2, CHCH2; X4 = piperidinyl, pyrrolidinyl, cycloalkyl, Ph, heteroaryl, or null; R1 = H, alkyl, amino, etc.; R2, R6 = H, Me; R3 = H, arylacyl, heteroarylacyl, arylalkylsulfonyl, etc.; R4 = H, alkyl or is absent if X2 is H; R5, R7, R8 = H, alkyl; R9 = CHO, COCF3, COCF2CF3, etc.; R10 = H, alkyl, amino, etc.; Y1, Y2 = O, H2; m, n, p, q = 0-4) and their pharmaceutically acceptable salts, prodrugs, etc. were prepared as inhibitors of factor Xa. The compds. are useful in vitro or in vivo for preventing or treating coagulation disorders. Thus, Boc-D-Arg-Gly-Arg-H (I, Boc = tert-butoxycarbonyl) was prepared from Boc-Arg(Z)-OH (Z = benzyloxycarbonyl), Boc-Gly-OH, and Boc-D-Arg(Z2)-OH via peptide couplings of arginine lactam intermediates. Peptide I was evaluated for biol. half-life, antithrombotic efficacy, and effects on hemostasis and hematomol. parameters.

IT 186369-07-3P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of peptides as inhibitors of factor Xa)

RN 186369-07-3 CAPLUS

CN Glycinamide, N2-[1,4-dioxo-4-(phenylmethoxy)butyl]-N5-

[imino[[(phenylmethoxy) carbonyl] amino]methyl]-N5-

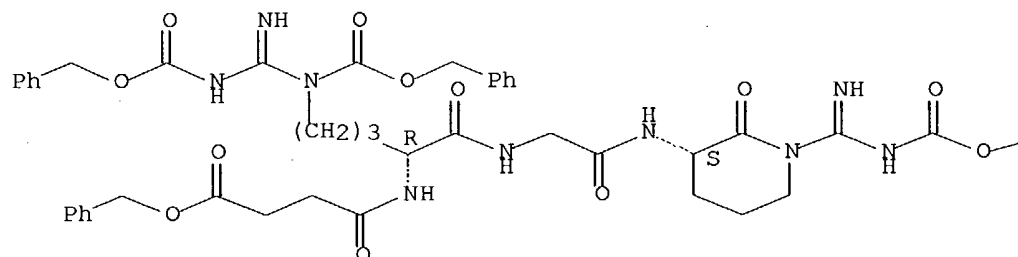
[(phenylmethoxy) carbonyl]-

D-ornithyl-N-[(3S)-1-[imino[[(phenylmethoxy) carbonyl] amino]methyl]-2-oxo-3-

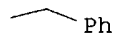
piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

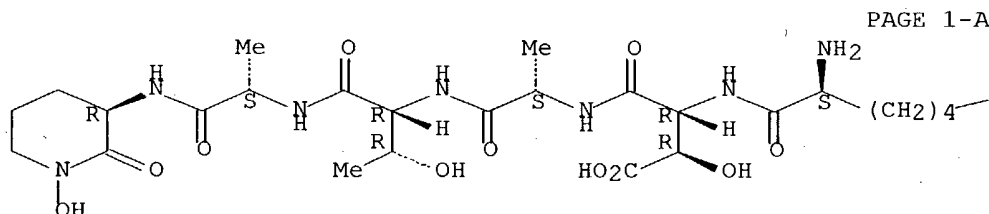


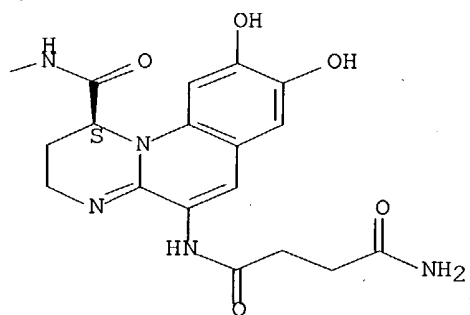
PAGE 1-B



L14 ANSWER 35 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:600816 CAPLUS Full-text
 DN 125:301560
 TI Synthesis of optically pure chrysobactin and immunoassay development
 AU Lu, Chuang; Buyer, Jeffrey S.; Okonya, John F.; Miller, Marvin J.
 CS Soil Microbial Systems Laboratory, US Department of Agriculture,
 Beltsville, MD, 20705-2350, USA
 SO BioMetals (1996), 9(4), 377-383
 CODEN: BOMEEH; ISSN: 0966-0844
 PB Rapid Science Publishers
 DT Journal
 LA English
 AB Chrysobactin [N-(2,3-dihydroxybenzoyl)-D-lysyl-L-serine], a siderophore
 that is essential for systemic virulence by plant pathogenic *Erwinia*
chrysanthemi, was synthesized with high diastereomeric purity.
 Chrysobactin was prepared by coupling of N α -(2,3-dibenzyloxybenzoyl)-
 N ϵ -benzyloxycarbonyl-D-lysine N-hydroxysuccinimide ester with L-serine
 benzyl ester followed by deprotection via hydrogenolysis. Optically pure
 chrysobactin was obtained with 98% overall yield. A monoclonal antibody
 to ferric chrysobactin was developed and characterized as IgM. The
 antibody reacts with chrysobactin, ferric chrysobactin and less strongly
 with ferric dihydroxybenzoic acid. The antibody reacts weakly with the
 siderophores ferrichrome, ferrichrome A, ferric pseudobactin and ferric
 rhodotorulic acid. This antibody was used in a competitive immunoassay
 to detect ferric chrysobactin at 10⁻⁸ to 10⁻¹⁰ mol. This immunoassay
 may provide a useful method for the detection of chrysobactin in plant
 samples.
 IT **76975-04-7**, Pseudobactin
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
 (Biological study); PROC (Process)
 (preparation of chrysobactin and conjugation to protein carriers for
 antibody and immunoassay development)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-
 D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

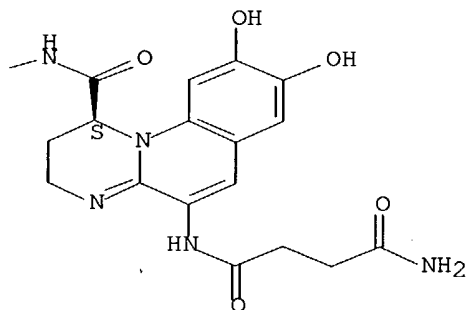
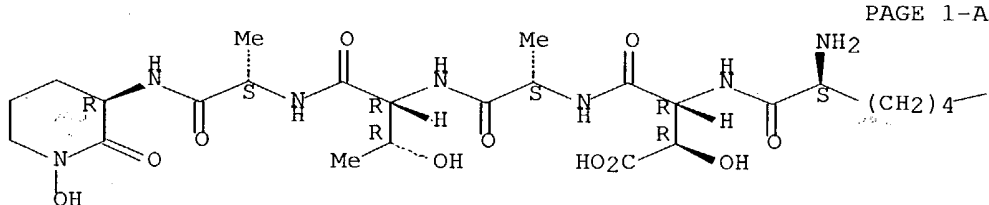
Absolute stereochemistry.





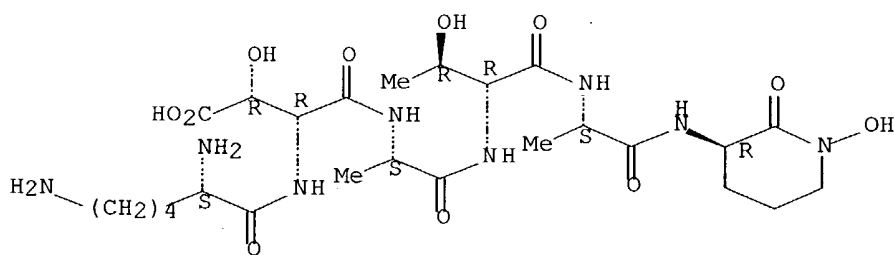
L14 ANSWER 36 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:405586 CAPLUS Full-text
 DN 125:168634
 TI Synthetic and biological studies of pseudobactin, analogs and peptide fragments of pseudobactin, and chrysobactin
 AU Okonya, John Francis
 CS Univ. of Notre Dame, Notre Dame, IN, USA
 SO (1996) 165 pp. Avail.: Univ. Microfilms Int., Order No. DA9619193
 From: Diss. Abstr. Int., B 1996, 57(2), 1090
 DT Dissertation
 LA English
 AB Unavailable
 IT **76975-04-7P**, Pseudobactin
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (analogs and peptide fragments; preparation and biol. studies of pseudobactin analogs and peptide fragments)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 37 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:339996 CAPLUS Full-text
 DN 125:115115
 TI Synthesis of fragments of the peptide component of pseudobactin
 AU Okonya, John F.; Kolasa, Teodozyj; Miller, Marvin J.
 CS Department Chemistry Biochemistry, University Notre Dame, Notre Dame,
 IN, USA
 SO Journal of Peptide Science (1996), 2(3), 157-164
 CODEN: JPSIEI; ISSN: 1075-2617
 PB Wiley
 DT Journal
 LA English
 AB Pseudobactin is a structurally complex and physiol. important
 siderophore (microbial iron chelator) from *Pseudomonas putida*-
fluorescens. Various fragments of the unusual peptide component of
 pseudobactin were prepared by solution-phase peptide synthesis. A class
 of related peptides named pseudomycins have shown promising antifungal
 activity. To examine if these peptide fragments above would elicit
 similar activity, the fragments were tested and found to have no
 antifungal activity in limited bioassays.
 IT **162553-96-0**
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); BIOL (Biological study)
 (preparation and antifungal activity of pseudobactin peptide
 fragments)
 RN 162553-96-0 CAPLUS
 CN L-Alaninamide, L-lysyl-threo-3-hydroxy-D- α -aspartyl-L-alanyl-D-
 allothreonyl-N-(1-hydroxy-2-oxo-3-piperidiny)-, (R)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



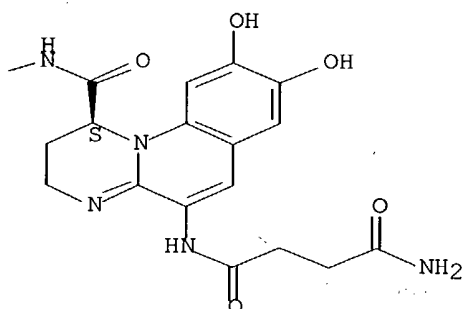
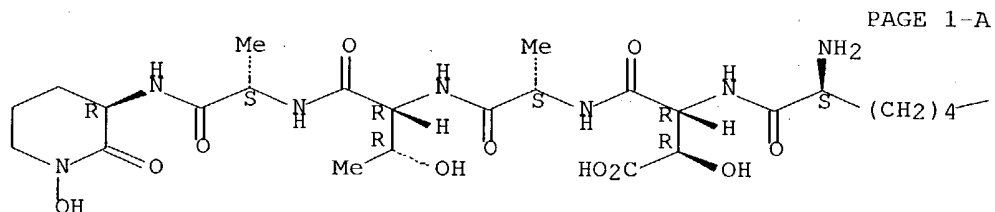
IT **76975-04-7DP**, Pseudobactin, peptide fragments **178858-99-6P**
178859-01-3P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological
 study, unclassified); SPN (Synthetic preparation); BIOL (Biological
 study); PREP (Preparation)
 (preparation and antifungal activity of pseudobactin peptide
 fragments)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-

8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

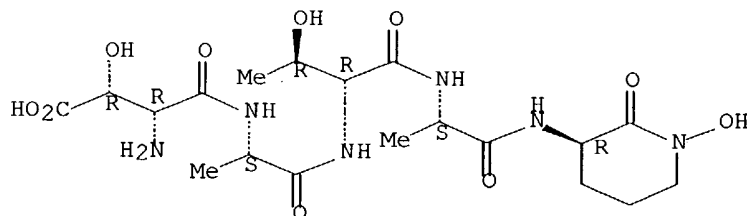
Absolute stereochemistry.



RN 178858-99-6 CAPLUS

CN L-Alaninamide, threo-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, (R)- (9CI) (CA INDEX NAME)

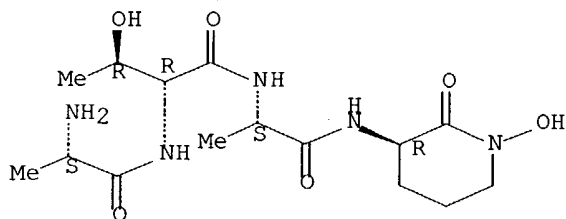
Absolute stereochemistry.



RN 178859-01-3 CAPLUS

CN L-Alaninamide, L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



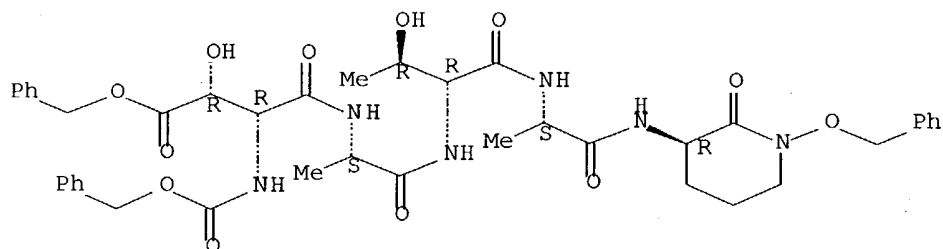
IT 178858-94-1P 178858-95-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent) (preparation and antifungal activity of
 pseudobactin peptide fragments).

RN 178858-94-1 CAPLUS

CN L-Alaninamide, threo-3-hydroxy-N-[(phenylmethoxy)carbonyl]-D- α -
 aspartyl-L-alanyl-D-allothreonyl-N-[2-oxo-1-(phenylmethoxy)-3-
 piperidinyl]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

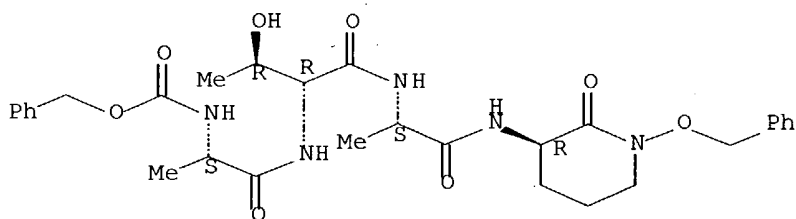
Absolute stereochemistry.



RN 178858-95-2 CAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-D-allothreonyl-N-[2-
 oxo-1-(phenylmethoxy)-3-piperidinyl]-, (R)- (9CI) (CA INDEX NAME)

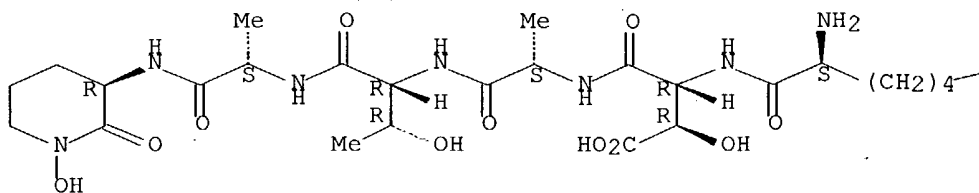
Absolute stereochemistry.



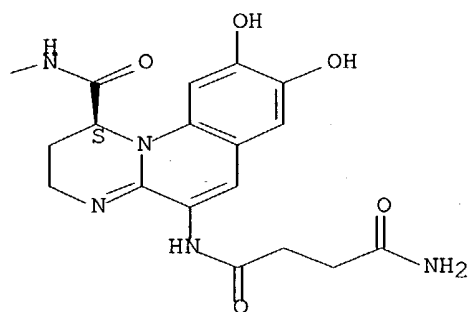
L14 ANSWER 38 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:163527 CAPLUS Full-text
 DN 124:226897
 TI Iron availability affects induction of systemic resistance to fusarium wilt of radish by *Pseudomonas fluorescens*
 AU Leeman, M.; Ouden, F. M. Den; Van Pelt, J. A.; Dirkx, F. P. M.; Steijl, H.; Bakker, P. A. H. M.; Schippers, B.
 CS Department Plant Ecology and Evolutionary Biology, Utrecht University, Utrecht, 3508 TB, Neth.
 SO Phytopathology (1996), 86(2), 149-55
 CODEN: PHYTAJ; ISSN: 0031-949X
 PB American Phytopathological Society
 DT Journal
 LA English
 AB A special bioassay on rock wool was used to study the influence of iron availability on the induction of systemic resistance in radish (*Raphanus sativus* L.) against *Fusarium* wilt mediated by *Pseudomonas fluorescens*. In this bioassay, the pathogen (*Fusarium oxysporum* f. sp. *raphani*) and a strain of *Pseudomonas*, salicylic acid (SA), or a pseudobactin were applied at sep. locations on the plant root. Strain WCS374 of *P. fluorescens* and its pseudobactin-minus Tn5 mutant gave greater disease control in the induced systemic resistance bioassay when iron availability in the radish nutrient solution was low than when it was high. Mutants of *P. fluorescens* strains WCS374 and WCS417 lacking the O-antigenic side chain of the lipopolysaccharide induced resistance at low but not at high iron availability. The purified pseudobactin of strain WCS374, but not the pseudobactins of strains WCS358 and WCS417, induced resistance. Gas chromatog. and spectrophotometry were used to detect and measure production of SA by these strains. Strains WCS374 and WCS417 produced 47 and 8 µg of SA per mL, resp., at low iron availability in vitro; the production of SA decreased rapidly with increasing iron availability. *P. putida* WCS358 did not induce resistance, either at low or at high iron availability, and did not produce SA in vitro. Com. SA induced resistance at concns. as low as 100 fg per root. High concns. (> 1 mg/mL) of SA reduced growth of hyphae from germinated conidia of *F. oxysporum* f. sp. *raphani*. We hypothesize that the Fe³⁺-chelating SA, produced by selected *P. fluorescens* strains at low iron availability, is involved in the induction of systemic resistance to *Fusarium* wilt of radish. The pseudobactin produced by WCS374 may be involved as well. Given these results, it seems appropriate to reevaluate the role of siderophore-mediated competition for iron in the suppression of disease by fluorescent *Pseudomonas* spp.
 IT **76975-04-7**, Pseudobactin
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (iron effect on *Pseudomonas fluorescens* production of)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L14 ANSWER 39 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:114637 CAPLUS Full-text

DN 124:167398

TI Transcriptional regulation of the iron-responsive sigma factor gene pbrA

AU Sexton, Ray; Gill, Paul R., Jr.; Dowling, David N.; O'Gara, Fergal

CS Microbiology Dep., Univ. College, Cork, Ire.

SO Molecular & General Genetics (1996), 250(1), 50-8

CODEN: MGGEAE; ISSN: 0026-8925

PB Springer

DT Journal

LA English

AB In response to the intracellular iron concentration *Pseudomonas fluorescens* M114 coordinately regulates the production of pseudobactin M114, its cognate receptor PbuA, and a casein protease. Transcriptional initiation of this coordinate iron-stress response requires the sigma factor PbrA. PbrA is a member of the ECF (Extracytoplasmic function) subgroup of the $\sigma 70$ family of eubacterial RNA polymerase sigma factors. Regulatory studies of the pbrA gene utilizing promoter-lacZ transcriptional fusions demonstrate that expression of pbrA dictates the cellular response to iron. PbrA is transcribed in all phases of iron-limited growth but maximally at late-logarithmic to stationary phase. PbrA expression is independent of autoregulatory control but is strictly repressed in iron-rich conditions in a Fur-dependent fashion. Constitutive expression of pbrA from an inducible tac promoter permits the induction of PbrA-dependent transcription and pseudobactin M114 biosynthesis in high-iron conditions. A PbrA consensus sequence was derived from significant DNA sequence homologies observed within the "-25 bp" and "-16 bp" regions conserved among all PbrA-dependent promoters. The predicted PbrA target promoter consensus is homologous for the promoter recognition sites for other environmentally responsive ECF sigma factors.

IT **76975-04-7**, Pseudobactin

RL: BSU (Biological study, unclassified); MFM (Metabolic formation);

BIOL

(Biological study); FORM (Formation, nonpreparative)

(M114; constitutive expression of pbrA from an inducible tac promoter permits the induction of PbrA-dependent transcription and

pseudobactin

M114 biosynthesis in high-iron conditions)

RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-

8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

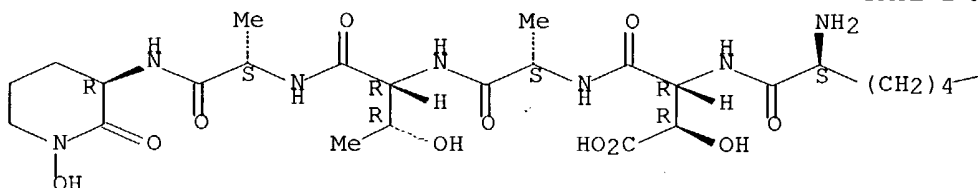
hydroxy-

D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-

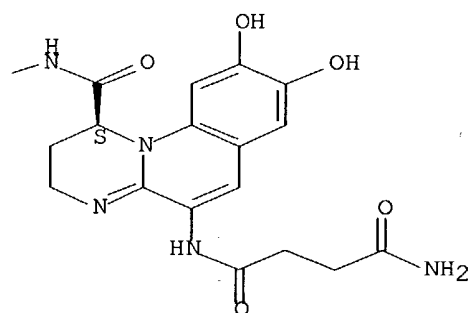
piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

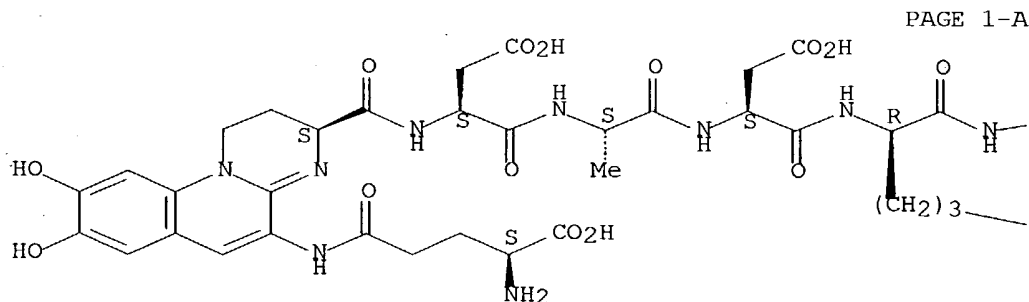


PAGE 1-B

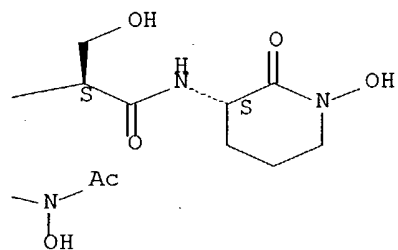


L14 ANSWER 40 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:954393 CAPLUS Full-text
 DN 124:283821
 TI Structure and characterization of isopyoverdin from *Pseudomonas putida* BTP1 and its relation to the biogenetic pathway leading to pyoverdins
 AU Jacques, Ph.; Ongena, M.; Gwose, I.; Seinsche, D.; Schroeder, H.; Delfosse, Ph.; Thonart, Ph.; Taraz, K.; Budzikiewicz, H.
 CS Institut fuer Organische Chemie der Universitaet, Cologne, D-50939, Germany
 SO Zeitschrift fuer Naturforschung, C: Biosciences (1995), 50(9/10), 622-9
 CODEN: ZNCBDA; ISSN: 0341-0382
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA English
 AB Pyoverdin-type siderophores produced by six fluorescent *Pseudomonas* strains isolated from different rhizospheres were purified and characterized. The purified ferri-pyoverdins were tested for their ability to promote the growth of other strains grown under iron deficiency conditions. Only the one obtained from *P. putida* BTP1 did not act as a growth promoter. The structure of the BTP1 siderophore was elucidated by spectroscopic methods and degradation studies. It turned out that it contains a chromophore which differs from the one typical for pyoverdins insofar as it carries the carboxyl group in 3- rather than in 1-position ((3S)-5-amino-1,2-dihydro-8,9-dihydroxy-3H-pyrimido[1,2-a]quinoline-3- carboxylic acid). The amino group of the chromophore is substituted with the 5-carboxyl group of L-glutamic acid and its carboxyl group with the N-terminus of the peptide L-Asp-L-Ala-L-Asp-D-N5-Ac-N5-OH-Orn-L-Ser-L-c-N5- OH-Orn. This isopyoverdin fits into the biogenic scheme which postulates ferribactins as the precursors of pyoverdins.
 IT **159325-01-6P**, Isopyoverdin
 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (structure and characterization of isopyoverdin from *Pseudomonas putida*)
 RN 159325-01-6 CAPLUS
 CN L-Serinamide, L-γ-glutamyl-(3S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinoline-3-carbonyl-L-α-aspartyl-L-alanyl-L-α-aspartyl-N5-acetyl-N5-hydroxy-D-ornithyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

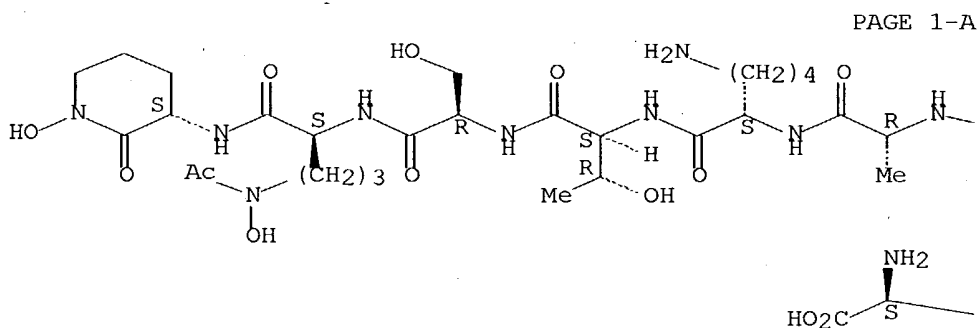


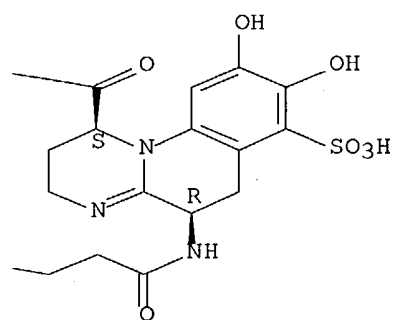
PAGE 1-B



L14 ANSWER 41 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:954392 CAPLUS Full-text
 DN 124:283820
 TI Dihydropyoverdin sulfonic acids - intermediates in biogenesis?
 AU Schroeder, H.; Adam, J.; Taraz, K.; Budzikiewicz, H.
 CS Institut fuer Organische Chemie, Universitaet zu Koeln, Cologne, D-50939,
 Germany
 SO Zeitschrift fuer Naturforschung, C: Biosciences (1995), 50(9/10), 616-21
 CODEN: ZNCBDA; ISSN: 0341-0382
 PB Verlag der Zeitschrift fuer Naturforschung
 DT Journal
 LA German
 AB From the culture media of Pseudomonas aptata 4b and of Pseudomonas fluorescens ATCC 13525 5,6-dihydropyoverdin-7-sulfonic acids could be isolated. Their possible role in the biogenetic pathway leading to the pyoverdins is discussed.
 IT **175526-87-1P**
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (dihydropyoverdin sulfonic acids of Pseudomonas as possible intermediates in pyoverdin biogenesis)
 RN 175526-87-1 CAPLUS
 CN L-Ornithinamide, N-[[5-[(4-amino-4-carboxy-1-oxobutyl)amino]-2,3,5,6-tetrahydro-8,9-dihydroxy-7-sulfo-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-
 D-alanyl-L-lysyl-L-threonyl-D-seryl-N5-formyl-N5-hydroxy-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1[1S-[1 α ,5 α (R*)]],5(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L14 ANSWER 42 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:852768 CAPLUS Full-text

DN 123:249335

TI Isolation, purification, characterization and partial structure determination of pseudobactins from *Pseudomonas putida* WCS358, ATCC 39167

and *Pseudomonas fluorescens* A225 and pseudobactin mediated iron transport

studies in these three *Pseudomonas* (siderophore)

AU Khalil, Safia

CS Univ. of Oklahoma, Norman, OK, USA

SO (1994) 310 pp. Avail.: Univ. Microfilms Int., Order No. DA9522768

From: Diss. Abstr. Int., B 1995, 56(3), 1390

DT Dissertation

LA English

AB Unavailable

IT **76975-04-7P**, Pseudobactin

RL: BSU (Biological study, unclassified); PRP (Properties); PUR

(Purification or recovery); BIOL (Biological study); PREP (Preparation)

(purification and properties and iron transport by pseudobactins from *Pseudomonas*)

RN 76975-04-7 CAPLUS

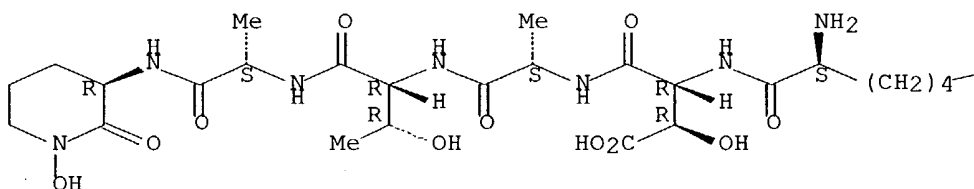
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

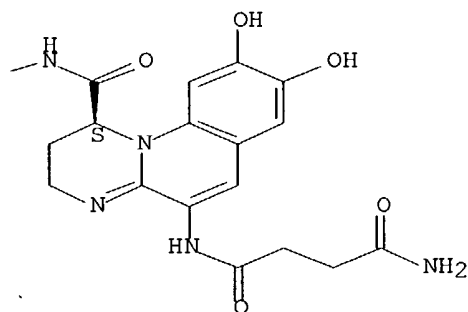
hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

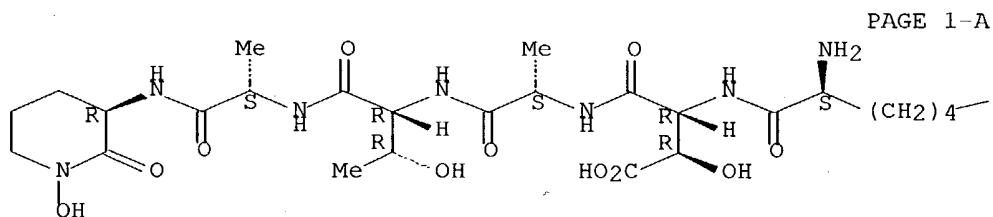


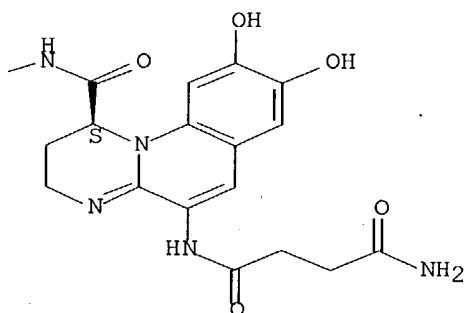
PAGE 1-B



L14 ANSWER 43 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:465848 CAPLUS Full-text
 DN 122:265982
 TI Synthesis of the Peptide Fragment of Pseudobactin
 AU Okonya, John F.; Kolasa, Teodozj; Miller, Marvin J.
 CS Department of Chemistry and Biochemistry, University of Notre Dame,
 Notre Dame, IN, 46556, USA
 SO Journal of Organic Chemistry (1995), 60(7), 1932-5
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 OS CASREACT 122:265982
 AB Synthesis of the peptide fragment H-L-Lys-D-threo- β -OH-Asp-L-Ala-D-allo-Thr-L-Ala-N-OH-D-cyclo-Orn of pseudobactin is reported. Using EEDQ as a coupling reagent, peptide bonds were constructed without requiring protection of hydroxyl groups. To access the D-allo-Thr residue in the peptide fragment of pseudobactin, the Thr residue in Cbz-L-Ala-D-Thr-L-Ala-OCMe₃ (Cbz = PhCH₂O₂C) was converted to a peptidyl oxazoline using Burgess' reagent. Hydrolysis of the oxazoline with 1 N HCl followed by base-catalyzed acyl migration then provided the D-allo-Thr analog.
 IT **76975-04-7P**, Pseudobactin
 RL: PNU (Preparation, unclassified); PREP (Preparation)
 (preparation of pseudobactin peptide fragment)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allo-threonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





IT 162553-90-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

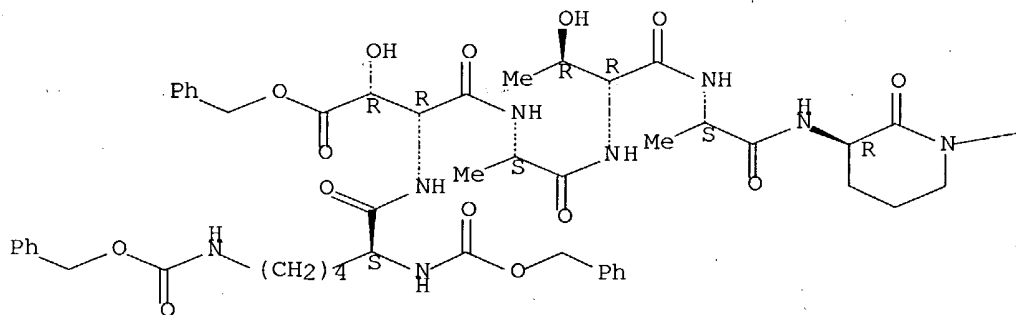
(preparation of pseudobactin peptide fragment)

RN 162553-90-4 CAPLUS

CN L-Alaninamide, N2,N6-bis[(phenylmethoxy)carbonyl]-L-lysyl-threo-3-hydroxy-

D- α -aspartyl-L-alanyl-D-allothreonyl-N-[2-oxo-1-(phenylmethoxy)-3-piperidiny]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



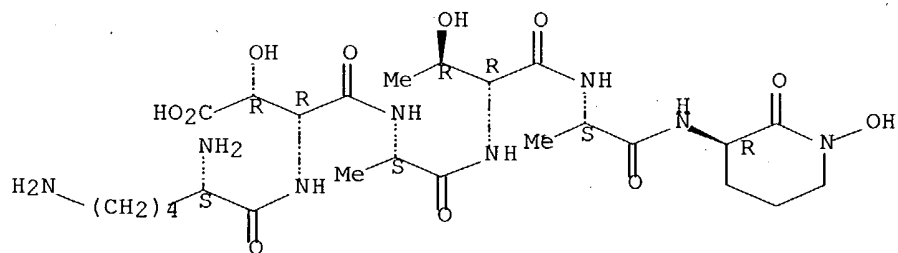
IT 162553-96-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pseudobactin peptide fragment)

RN 162553-96-0 CAPLUS

CN L-Alaninamide, L-lysyl-threo-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidiny)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L14 ANSWER 44 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:374251 CAPLUS Full-text

DN 122:155405

TI Isolation and analysis of the iron-free siderophore, pseudobactin by semipreparative LC on a polymeric stationary phase

AU Glennon, J. D.; Manley, K.; Ruangviriyachai, C.; O'Gara, F.; Budzikiewicz,

H.

CS Chemistry Dep., Univ. College Cork, UK

SO International Journal of Bio-Chromatography (1994), 1(1), 57-67

CODEN: IJOBEQ; ISSN: 1068-0659

PB Harwood

DT Journal

LA English

AB The isolation of the yellow-green fluorescent siderophore, Pseudobactin, produced by selected Pseudomonas species in culture media, can be carried out by medium pressure liquid chromatog. of the Fe(III) complex using 5-20 μ m LiChroprep RP-18. Detection is achieved using either uv (220 nm) or visible (405 nm) wavelength settings for the Fe(III)-pseudobactin and free pseudobactin species. Fluorescence detection however is selective for the free or uncomplexed pseudobactin and is used to monitor the production of the siderophore in bacterial culture media. An alternative isolation procedure, involving semi-preparative chromatog. on a polymeric PLRP-S column using a metal-free LC system, is shown to be an effective method for obtaining the free siderophore, avoiding the need for a decomplexation step.

IT 76975-04-7, Pseudobactin

RL: ANT (Analyte); ANST (Analytical study)

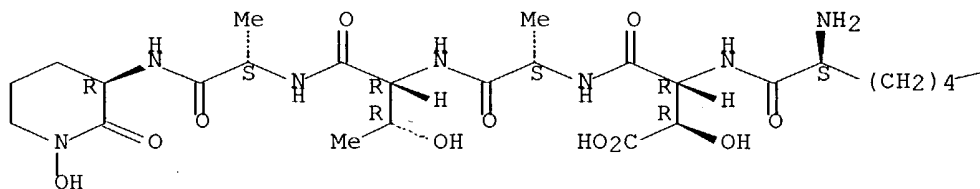
(isolation and anal. of the iron-free siderophore, pseudobactin by semipreparative LC on a polymeric stationary phase)

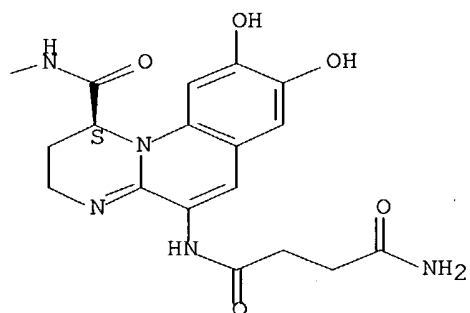
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





L14 ANSWER 45 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:361941 CAPLUS Full-text

DN 122:307762

TI Iron-responsive gene expression in *Pseudomonas fluorescens* M114: cloning and characterization of a transcription-activating factor, PbrA

AU Sexton, Ray; Gill, Paul R., Jr.; Callanan, Michael J.; O'Sullivan, Daniel

J.; Dowling, David N.; O'Gara, Fergal

CS Department Microbiology, University College Cork, Ire.

SO Molecular Microbiology (1995), 15(2), 297-306

CODEN: MOMIEE; ISSN: 0950-382X

PB Blackwell

DT Journal

LA English

AB In response to iron limitation, *Pseudomonas fluorescens* M114 induces a number of genes including an iron-scavenging siderophore termed pseudobactin M114, its cognate receptor, PbuA, and a casein protease. A Tn5lacZ-induced mutant (M114FA1) was isolated that exhibits a pleiotropic phenotype and lacks the ability to express these iron-regulated genes. A cosmid clone was identified which complements this mutation. This clone is capable of activating a number of iron-regulated promoter fusion constructs from *P. fluorescens* M114 and *Pseudomonas putida* WCS358 and can also promote expression of these fusions in *Escherichia coli*. A series of insertion mutants was constructed by homologous recombination which were unable to transcribe the promoter fusions. DNA sequence anal. of the complementing region identified one open reading frame (ORF) termed pbrA (pseudobactin regulation activation) and the deduced amino acid shows domains with significant homol. to a number of ECF (extracytoplasmic function) transcriptional regulators of the $\sigma 70$ sigma factor family, including fecI required for expression of the ferric dicitrate outer-membrane receptor protein of *E. coli*. Sequences upstream of the pbrA gene suggest that transcription of pbrA may also be iron regulated.

IT 76975-04-7, Pseudobactin

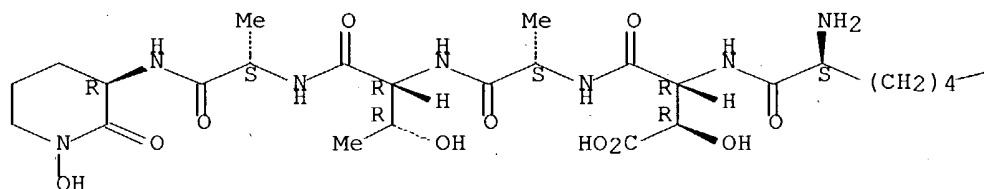
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(iron-responsive gene pbrA-encoded protein of *Pseudomonas fluorescens* M114 regulating)

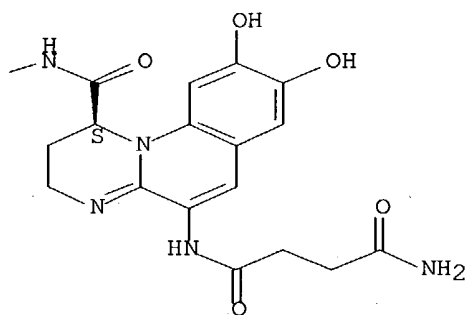
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

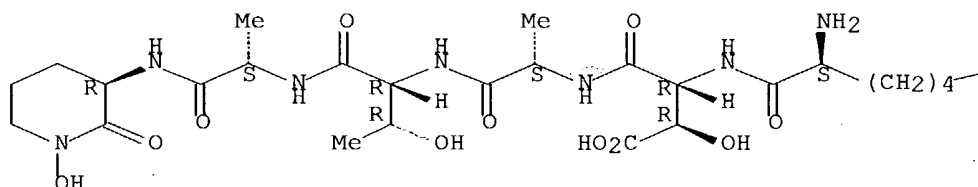


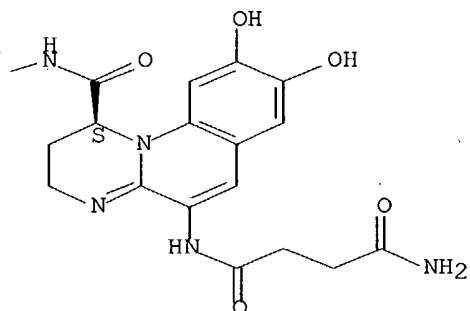


L14 ANSWER 46 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:197915 CAPLUS Full-text
 DN 122:29808
 TI Isolation strategy for identifying bioactive compounds from fermentation broth
 AU Bortolo, Rossella; Andriollo, Nunzio; Cauchi, Emanuele; Cassani, Giorgio
 CS Enichem Istituto G. Donegani, Novara, Italy
 SO Special Publication - Royal Society of Chemistry (1994), 158 (Separations for Biotechnology 3), 60-6
 CODEN: SROCD0; ISSN: 0260-6291
 DT Journal
 LA English
 AB Some 5300 soil microbial strains were screened for the identification of potentially new fungicides, insecticides, and herbicides. Subsequent fermns. led to the isolation of 40 bioactive compds. which could be separated into 6 broad categories: macrolides, macrocycles, polyenes, anthracyclines, nucleosides, and miscellaneous
 IT **76975-04-7P**, Pseudobactin **159650-21-2P**, Pseudobactin B
 RL: PRP (Properties); PUR (Purification or recovery); PREP (Preparation) (pseudobactin and pseudobactin B from Pseudomonas)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

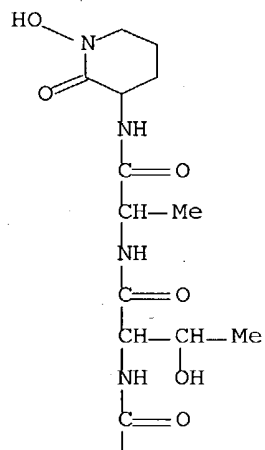




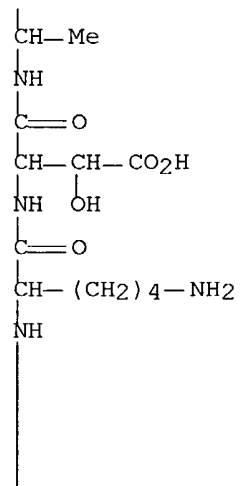
RN 159650-21-2 CAPLUS

CN L-Alaninamide, N2-[[5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-erythro-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidiny)-
(9CI)

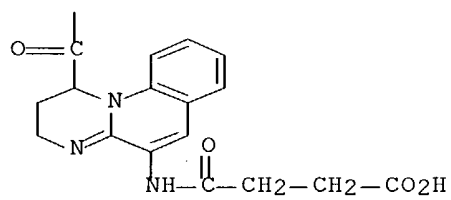
(CA INDEX NAME)



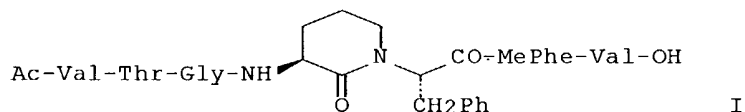
PAGE 2-A



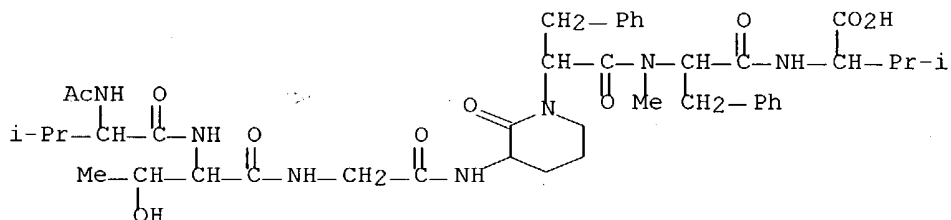
PAGE 3-A



L14 ANSWER 47 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:66982 CAPLUS Full-text
 DN 122:10607
 TI In situ synthesis of δ -lactams in continuous flow SPPS
 AU Hone, Neal D.; Chhabra, Siri Ram; Bycroft, Barrie W.
 CS Dep. Pharmaceuticals Sci., Univ. Nottingham, Nottingham, NG7 2RD, UK
 SO Pept. 1992, Proc. Eur. Pept. Symp., 22nd (1993), Meeting Date 1992, 292-
 3. Editor(s): Schneider, Conrad H.; Eberle, Alex N. Publisher: ESCOM,
 Leiden, Neth. CODEN: 60LUAN
 DT Conference
 LA English
 GI



AB A report from a symposium on the preparation of peptidyl δ -lactams, e.g.
 I, via solid-phase peptide synthesis (SPPS) procedures.
 IT **159585-57-6P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (in situ synthesis of peptidyl δ -lactams in continuous flow
 solid-phase peptide synthesis)
 RN 159585-57-6 CAPLUS
 CN L-Valine, N-[N-[2-[3-[[N-[N-(N-acetyl-L-valyl)-L-threonyl]glycyl]amino]-
 2-oxo-1-piperidinyl]-1-oxo-3-phenylpropyl]-N-methyl-L-phenylalanyl]-,
 [S-(R*,R*)]- (9CI) (CA INDEX NAME)



L14 ANSWER 48 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:46710 CAPLUS Full-text

DN 122:48016

TI Isolation of a gene (pbsC) required for siderophore biosynthesis in fluorescent *Pseudomonas* sp. strain M114

AU Adams, Claire; Dowling, David N.; O'Sullivan, Dan J.; O'Gara, Fergal

CS Microbiol. Dep., Univ. Coll., Cork, Ire.

SO Molecular and General Genetics (1994), 243(5), 515-524

CODEN: MGGEAE; ISSN: 0026-8925

DT Journal

LA English

AB An iron-regulated gene, pbsC, required for siderophore production in fluorescent *Pseudomonas* sp. strain M114 has been identified. A kanamycin-resistance cassette was inserted at specific restriction sites within a 7 kb genomic fragment of M114 DNA and by marker exchange two siderophore-neg. mutants, designated M1 and M2, were isolated. The nucleotide sequence of approx. 4 kb of the region flanking the insertion sites was determined and a large open reading frame (ORF) extending for 2409 bp was identified. This gene was designated pbsC (pseudobactin synthesis C) and its putative protein product termed PbsC. PbsC was homologous to a family of enzymes involved in the biosynthesis of secondary metabolites, including EntF of *Escherichia coli*. These enzymes are believed to act via ATP-dependent binding of AMP to their substrate. Several areas of high sequence homol. between these proteins and PbsC were observed, including a conserved AMP-binding domain. The expression of pbsC is iron-regulated as revealed when a DNA fragment containing the upstream region was cloned in a promoter probe vector and conjugated into the wild-type strain, M114. The nucleotide sequence upstream of the putative translational start site contains a region homologous to previously defined -16 to -25 sequences of iron-regulated genes but did not contain an iron-box consensus sequence. It was noted that inactivation of the pbsC gene also affected other iron-regulated phenotypes of *Pseudomonas* M114.

IT 76975-04-7, Pseudobactin

RL: FORM (Formation, nonpreparative)

(formation of, *Pseudomonas* gene pbsC required for, nucleotide sequence of)

RN 76975-04-7 CAPLUS

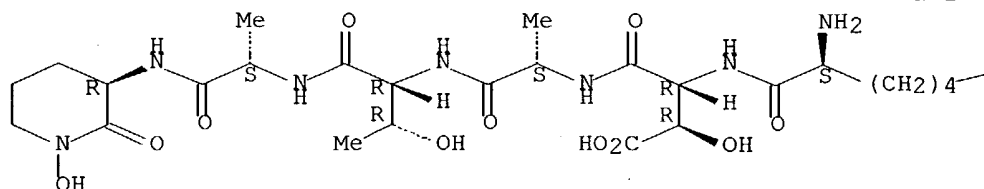
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

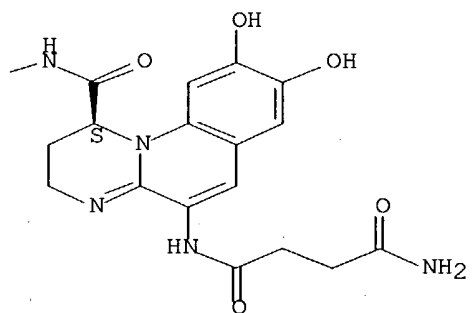
D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L14 ANSWER 49 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:33954 CAPLUS Full-text
 DN 122:5030
 TI Bacterial constituents. LVIII. Isopyoverdin Pp BTP 1, a biogenetically interesting novel siderophore from *Pseudomonas putida*
 AU Jacques, P.; Gwose, I.; Seinsche, D.; Taraz, K.; Budzikiewicz, H.; Schroeder, H.; Ongena, M.; Thonart, P.
 CS Institut Organische Chemie, Universitat Koeln, Cologne, D-50939, Germany
 SO Natural Product Letters (1993), 3(3), 213-18
 CODEN: NPLEEF; ISSN: 1057-5634
 DT Journal
 LA English
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A siderophore was isolated from *Pseudomonas putida* BTP 1 cultures; this siderophore contains the chromophore I rather than II typical for pyoverdins. Its structure was elucidated by mass spectrometry, NMR and chemical degradation. This new structural type is of great interest: the currently accepted biogenetic pathway leading to II starts from D-Tyr and L-2,4-diaminobutyric acid (Dab) which condense to give the ferribactin chromophore III. Subsequent ring closure via the α -nitrogen of Dab leads to II, while the alternative ring closure via the γ -nitrogen would yield I. The structure of the new siderophore was confirmed as IV. This is for the first time that this isochromophore has been detected in a *Pseudomonas* siderophore. Its discovery confirms the assumed intermediacy of ferribactins in the biogenesis of pyoverdins.

IT 159325-01-6 159325-01-6D, iron complex

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

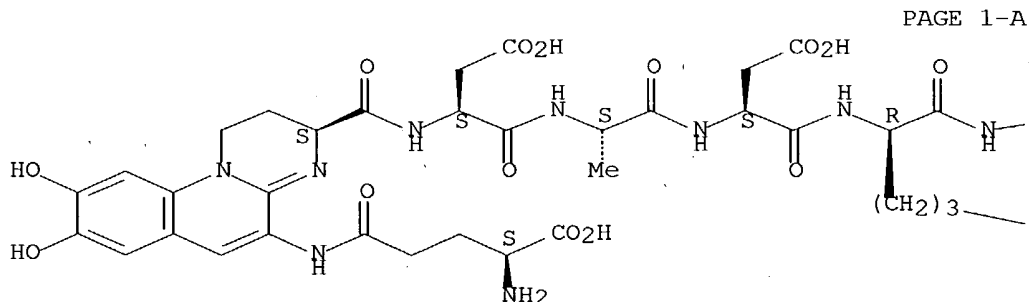
MFM

(Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence)
 (novel siderophore from *Pseudomonas putida*).

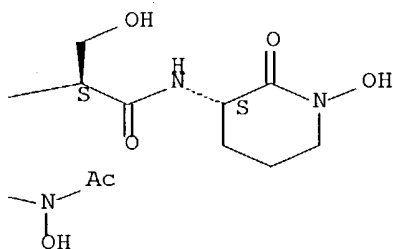
RN 159325-01-6 CAPLUS

CN L-Serinamide, L- γ -glutamyl-(3S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinoline-3-carbonyl-L- α -aspartyl-L-alanyl-L- α -aspartyl-N5-acetyl-N5-hydroxy-D-ornithyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-B

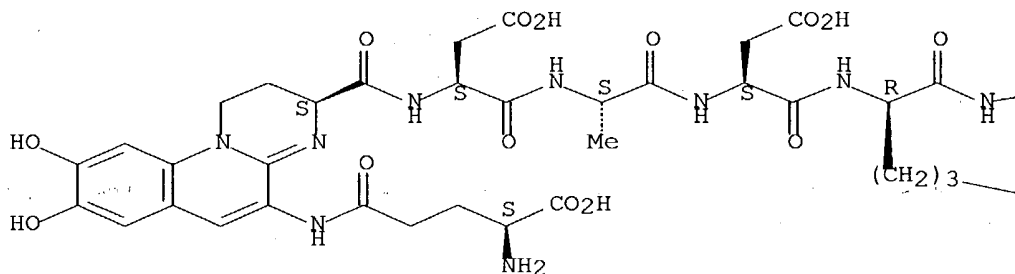


RN 159325-01-6 CAPLUS

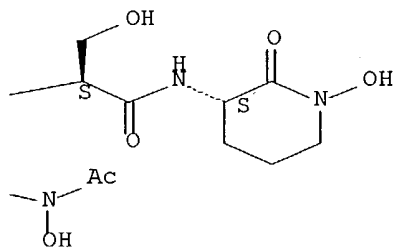
CN L-Serinamide, L-γ-glutamyl-(3S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinoline-3-carbonyl-L-α-aspartyl-L-alanyl-L-α-aspartyl-N5-acetyl-N5-hydroxy-D-ornithyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L14 ANSWER 50 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:12803 CAPLUS Full-text

DN 122:56486

TI Stability constants of pseudobactin complexes with transition metals

AU Chen, Yona; Jurkevitch, Edouard; Bar-Ness, Eli; Hadar, Yitzhak

CS Fac. Agric., Hebrew Univ. Jerusalem, Rehovot, 76100, Israel

SO Soil Science Society of America Journal (1994), 58(2), 390-6

CODEN: SSSJD4; ISSN: 0361-5995

DT Journal

LA English

AB The stability consts. of the fluorescent siderophore pseudobactin St3 (PSB3) produced by *Pseudomonas putida* strain 3 with Fe³⁺, Cu²⁺, Mn²⁺, Zn²⁺, and Fe²⁺ were determined using fluorescence spectroscopy and potentiometric titrns. Stability consts. for PSB3, with Fe³⁺, Fe²⁺, Mn²⁺, and Zn²⁺ were determined based on titration to saturation of a PSB3 ligand solution with either of the metals, then back-titrating the solution with an EDTA solution along with simultaneous measurements of fluorescence and visible spectra. A nonlinear curve fitting between the fluorescence intensity (Y) and the concentration (C) of the metal or EDTA was used for the determination of the concns. of the free and complexed ligands. The overall stability constant (log KML) obtained for Fe³⁺ by this method was the same as that obtained by visible spectroscopy. The log KML values obtained by fluorescence spectroscopy for Mn²⁺ and Zn²⁺ were in good agreement with those obtained by potentiometric titration. Two samples obtained from PSB3 solns. isolated and purified from cultures grown under different conditions chelated Fe³⁺ with practically the same affinity.

IT 76975-04-7D, Pseudobactin, transition metal complexes

RL: PRP (Properties)

(stability consts. of pseudobactin complexes with transition metals)

RN 76975-04-7 CAPLUS

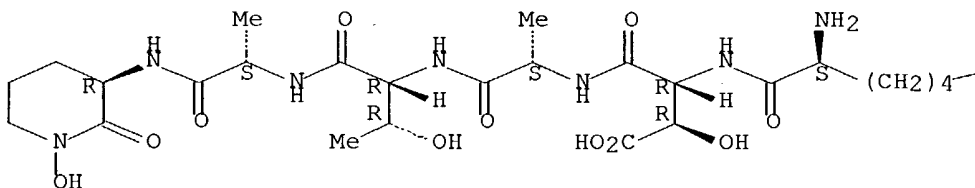
CN L-Alaninamide, N6-[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

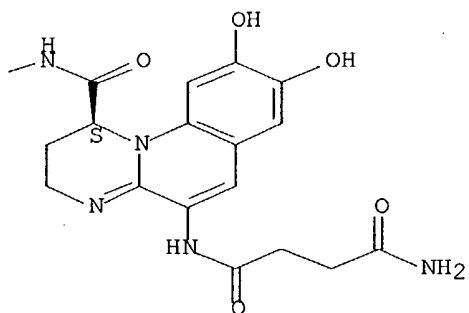
dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

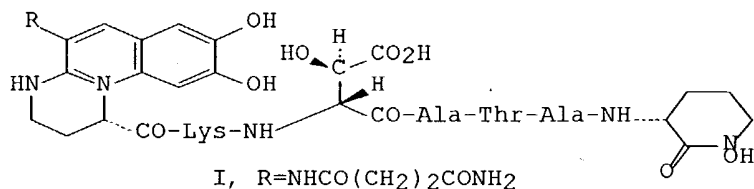
Absolute stereochemistry.

PAGE 1-A





L14 ANSWER 51 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1994:600640 CAPLUS Full-text
 DN 121:200640
 TI Biosynthesis of the pseudobactin chromophore from tyrosine
 AU Nowak-Thompson, Brian; Gould, Steven J.
 CS Dep. Chem., Oregon State Univ., Corvallis, OR, 97331-4003, USA
 SO Tetrahedron (1994), 50(33), 9865-72
 CODEN: TETRAB; ISSN: 0040-4020
 DT Journal
 LA English
 GI



AB Biosynthetic studies have shown the incorporation of DL-[2,3,3-²H₃]-tyrosine into the chromophore of pseudobactin (I), a siderophore produced by *Pseudomonas fluorescens* B10. A subsequent feeding using DL-[2',5',6'-²H₃]-3,4-dihydroxyphenylalanine showed no incorporation of the label, suggesting that oxidation of the aryl ring occurs after the incorporation of tyrosine. The ¹³C-NMR assignments of pseudobactin are also reported herein.

IT 76975-04-7, Pseudobactin

RL: FORM (Formation, nonpreparative)

(formation of, from tyrosine by *Pseudomonas fluorescens*)

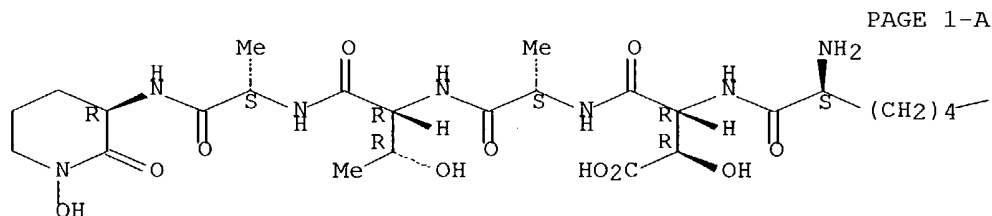
RN 76975-04-7 CAPLUS

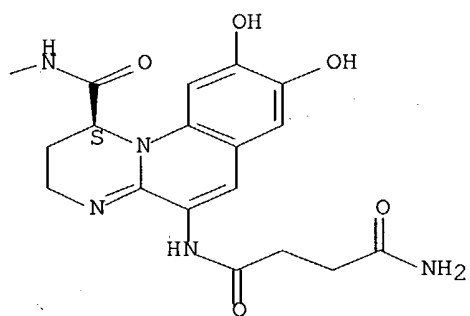
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L14 ANSWER 52 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:264955 CAPLUS Full-text

DN 120:264955

TI A simple assay for fluorescent siderophores produced by *Pseudomonas* species and an efficient isolation of pseudobactin

AU Nowak-Thompson, Brian; Gould, Steven J.

CS Dep. Chem., Oreg. State Univ., Corvallis, OR, USA

SO BioMetals (1994), 7(1), 20-4

CODEN: BOMEEH; ISSN: 0966-0844

DT Journal

LA English

AB Several iron binding metabolites (siderophores) of *Pseudomonas fluorescens* B10 (JL-3133) have been detected using C18 reverse phase HPLC coupled with photodiode array detection methods. This anal. utilized a volatile mobile phase of 90% 20 mM NH₄HCO₃/10% MeOH, pH 6.5. It has been shown to be applicable to other *P. fluorescens* strains for the detection of related metabolites. Direct scale-up of the anal. HPLC conditions allowed for the efficient preparative isolation of pseudobactin, the principle siderophore produced by *P. fluorescens* B10 (JL-3133).

IT 76975-04-7, Pseudobactin

RL: ANST (Analytical study)

(simple assay for fluorescent siderophores produced by *Pseudomonas* species and efficient isolation of)

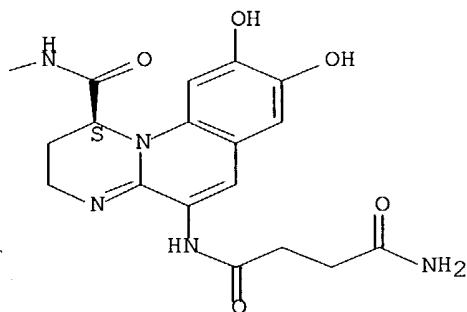
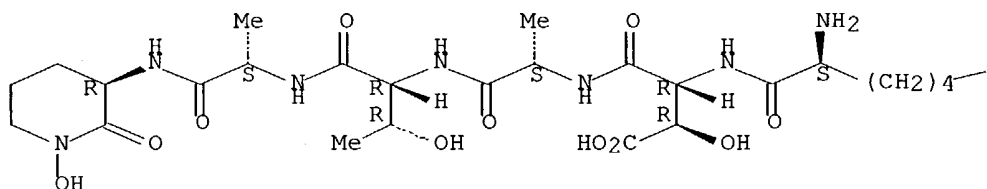
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 53 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:101604 CAPLUS Full-text

DN 120:101604

TI Indirect utilization of the phytosiderophore mugineic acid as an iron source to rhizosphere fluorescent *Pseudomonas*

AU Jurkevitch, Edouard; Hadar, Yitzhak; Chen, Yona; Chino, Mitsuo; Mori, Satoshi

CS Fac. Agric., Hebrew Univ. Jerusalem, Rehovot, Israel

SO BioMetals (1993), 6(2), 119-23

CODEN: BOMEEH; ISSN: 0966-0844

DT Journal

LA English

AB The phytosiderophore mugineic acid (MA) was studied as a source of Fe for rhizosphere fluorescent pseudomonads. ⁵⁵Fe supplied as Fe-MA was taken up by *Pseudomonas putida* WCS358, B10, and St3 grown under Fe deficient conditions. The uptake decreased when the bacteria were grown in the presence of Fe. However, no differences in uptake were observed when a siderophore-deficient mutant was tested. Since ligand exchange between pseudobactin and MA occurred rapidly, with a half-life of 2 h, MA-mediated Fe uptake probably proceeds through this indirect mechanism. The ecol. implications of these findings are discussed.

IT **76975-04-7**, Pseudobactin

RL: BIOL (Biological study)

(iron exchange between mugineic acid and)

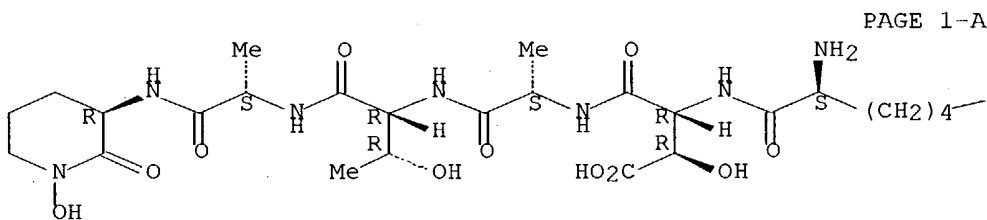
RN 76975-04-7 CAPLUS

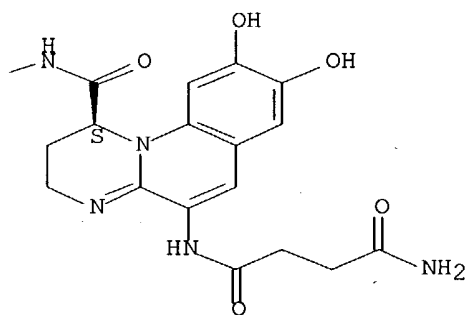
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

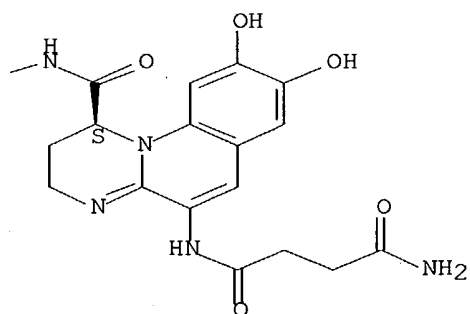
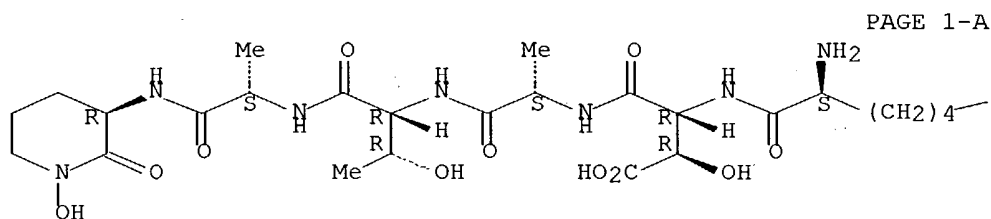
Absolute stereochemistry.





L14 ANSWER 54 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1994:27581 CAPLUS Full-text
 DN 120:27581
 TI Enhancement of symbiotic nitrogen fixation by vitamin-secreting
 fluorescent *Pseudomonas*
 AU Derylo, Mieczyslaw; Skorupska, Anna
 CS Dep. Gen. Microbiol., Univ. M. Curie-Sklodowska, Lublin, PL 20-033, Pol.
 SO Plant and Soil (1993), 154(2), 211-17
 CODEN: PLSOA2; ISSN: 0032-079X
 DT Journal
 LA English
 AB Fluorescent *Pseudomonas* sp. strain 267 promotes growth of nodulated
 clover plants under gnotobiotic conditions. In the growth conditions
 (60 μ M FeCl₃), the production of siderophores of the pseudobactin-
 pyoverdine group was repressed. Plant growth enhancement results from
 secretion of B vitamins by *Pseudomonas* sp. strain 267. This was proven
 by stimulation of clover growth by naturally auxotrophic strains of
Rhizobium leguminosarum bv. *trifolii* and marker strains *E. coli* thi⁻ and
R. meliloti pan⁻ in the presence of the supernatant of *Pseudomonas* sp.
 strain 267. The addition of vitamins to the plant medium increased
 symbiotic nitrogen fixation by the clover plants.
 IT **76975-04-7**, Pseudobactin
 RL: FORM (Formation, nonpreparative)
 (formation of, by fluorescent *Pseudomonas* secreting vitamins
 enhancing
 symbiotic nitrogen fixation in clover, iron effect on)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-
 D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

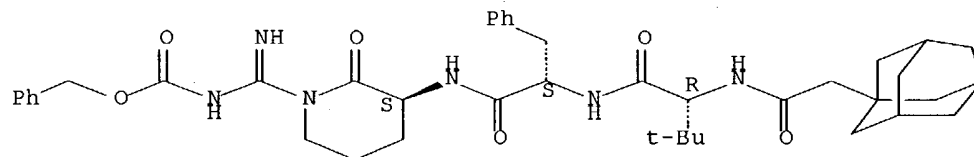
Absolute stereochemistry.



L14 ANSWER 55 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1993:626432 CAPLUS Full-text
 DN 119:226432
 TI Preparation of tripeptide derivatives as analgesics and
 antiinflammatories
 IN McIver, John McMillan
 PA Procter and Gamble Co., USA
 SO PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

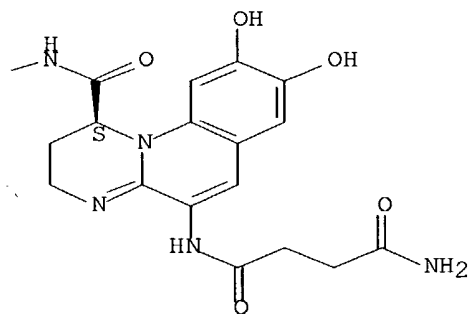
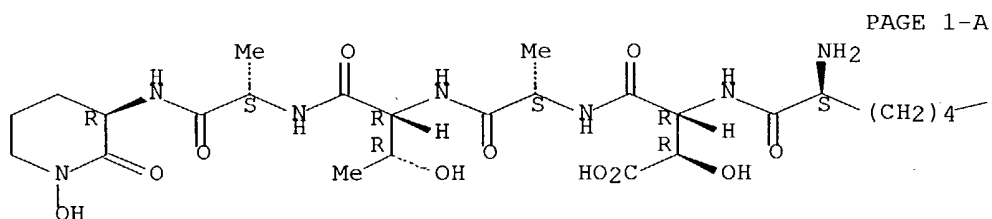
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9308211	A1	19930429	WO 1992-US8901	19921019
	W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, PL, RO, RU, SD				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
	AU 9228827	A1	19930521	AU 1992-28827	19921019
PRAI	US 1991-780607		19911023		
	WO 1992-US8901		19921019		
OS	MARPAT 119:226432				
AB	X(CH ₂) _n VZCHRCONHCHR1CONHCHR2COY [n = 0-2; R = (unsatd.) (cyclo)alkyl; R ₁ = R, aralkyl; R ₂ = (CH ₂) _m ANH ₂ , (CH ₂) _m ABC(:NH)NH ₂ ; m = 1-5; A = bond, p-phenylene, 1,4-cyclohexanediyl; B = bond, NH; Y = H, CF ₃ ; Z = O, NH; V = CO ₂ , NQCO, NQCS, CO, SO ₂ , P(O)(OH); X = (cyclo)alkyl, aryl; Q = H, (unsatd.) alkyl; QX = cyclic moiety; the carbon bearing R has the D- or L-configuration; the carbons bearing R ₁ , R ₂ have the L-configuration; with provisos], were prepared as an analgesics and antiinflammatories (no data). Thus, BOC-D-Phe-Phe-Arg-H.OAc was prepared via coupling of BOC-D-Phe-Phe-OH (preparation given) with N-carbobenzoyloxyamidino-2-aminovalerolactam.HCl (preparation given) using Et ₃ N/NCP(O)(OEt) ₂ in CH ₂ Cl ₂ followed by LiAlH ₄ reduction and hydrogenolysis over Pd/C. Dosages and formulations of specific title compds. are given.				
IT	150906-26-6P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for tripeptide analgesic and antiinflammatory)				
RN	150906-26-6 CAPLUS				
CN	L-Phenylalaninamide, 3-methyl-N-(tricyclo[3.3.1.1 ^{3,7}]dec-1-ylacetyl)-D-valyl-N-[(3S)-1-[imino[(phenylmethoxy)carbonyl]amino]methyl]-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)				

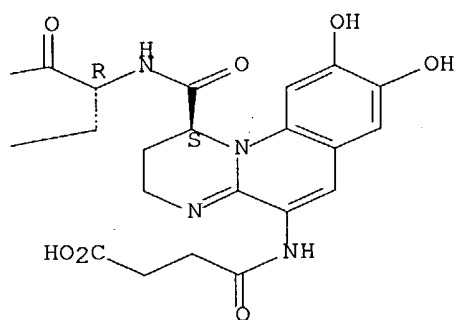
Absolute stereochemistry.



L14 ANSWER 56 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1993:534672 CAPLUS Full-text
 DN 119:134672
 TI Analysis of the microbial siderophore pseudobactin and its iron(III) complex by high-performance liquid chromatography with amperometric detection
 AU Manley, Keven; Ruangviriyachai, Chalerm; Glennon, Jeremy D.
 CS Chem. Dep., Univ. Coll. Cork, Cork, Ire.
 SO Analytical Proceedings (1993), 30(3), 154-6
 CODEN: ANPRDI; ISSN: 0144-557X
 DT Journal
 LA English
 AB The HPLC separation of pseudobactin and its Fe³⁺ complex on a polymeric column is reported together with the use of amperometric detection for analyses in culture media.
 IT **76975-04-7**
 RL: PROC (Process)
 (separation of, by HPLC with amperometric detection)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L14 ANSWER 58 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:187491 CAPLUS Full-text

DN 118:187491

TI A method for detection of pseudobactin, the siderophore produced by a plant-growth-promoting *Pseudomonas* strain, in the barley rhizosphere

AU Buyer, Jeffrey S.; Kratzke, Marian G.; Sikora, Lawrence J.

CS Soil Microbial Syst. Lab., USDA, Beltsville, MD, 20705-2350, USA

SO Applied and Environmental Microbiology (1993), 59(3), 677-81

CODEN: AEMIDF; ISSN: 0099-2240

DT Journal

LA English

AB Detection in the rhizosphere of the siderophore produced by an inoculated microorganism is critical to determining the role of microbial iron chelators on plant growth promotion. The development of monoclonal antibodies (MAb) to ferric pseudobactin, the siderophore of plant-growth-promoting *Pseudomonas* strain B10, was previously reported. One of these MAb reacted less strongly to pseudobactin than to ferric pseudobactin. The MAb reacted to Al(III), Cr(III), Cu(II), and Mn(II) complexes of pseudobactin at a level similar to the level at which it reacted to ferric pseudobactin and reacted less to the Zn(II) complex, but these metals would make up only a small fraction of chelated pseudobactin in soil on the basis of relative abundance of metals and relative binding consts. Fourteen-day-old barley plants grown in limed and autoclaved soil were inoculated with 10⁹ CFU of *Pseudomonas* strain Sml-3, a strain of *Pseudomonas* B10 Rif Nal selected for enhanced colonization, and sampled 3 days later. Extraction and anal. of the roots and surrounding soil using the MAb in an immunoassay indicated a concentration of 3.5 + 10⁻¹⁰ mol of ferric pseudobactin g⁻¹ (wet weight). This is the first direct measurement of a pseudobactin siderophore in soil or rhizosphere samples.

IT 76975-04-7D, metal complexes

RL: ANT (Analyte); ANST (Analytical study)

(detection of, in barley rhizosphere)

RN 76975-04-7 CAPLUS

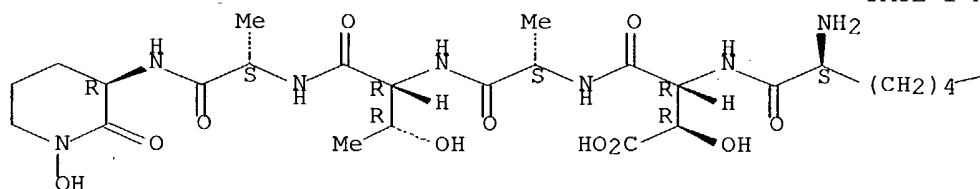
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

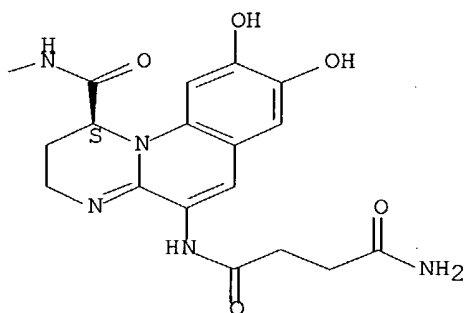
dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





IT 76975-04-7, Pseudobactin

RL: PROC (Process)

(from Pseudomonas, detection of, in barley rhizosphere)

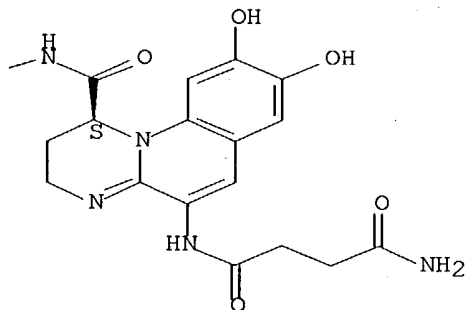
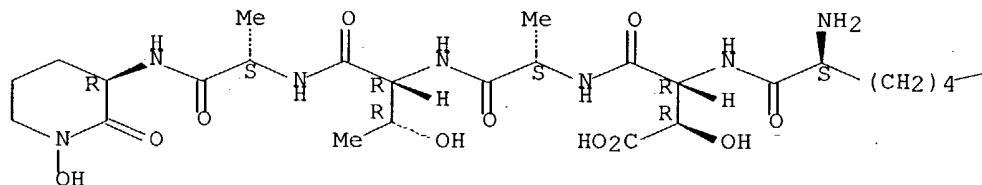
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 59 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:6238 CAPLUS Full-text

DN 118:6238

TI Short-term effects of rhizosphere microorganisms on iron uptake from microbial siderophores by maize and oat

AU Bar-Ness, Eli; Hadar, Yitzhak; Chen, Yona; Roemheld, Volker; Marschner, Horst

CS Fac. Agric., Hebrew Univ. Jerusalem, Rehovot, 76100, Israel

SO Plant Physiology (1992), 100(1), 451-6

CODEN: PLPHAY; ISSN: 0032-0889

DT Journal

LA English

AB Effects of rhizosphere microorganisms on Fe uptake by oat (*Avena sativa*) and maize (*Zea mays*) were studied in short-term (10 h) nutrient solution expts. Fe was supplied either as microbial siderophores (pseudobactin [PSB] or ferrioxamine B [FOB]) or as phytosiderophores obtained as root exudates from barley (epi-3-hydroxy-mugineic acid [HMA]) under varied population densities of rhizosphere microorganisms (axenic, uninoculated, or inoculated with different microorganism cultures). When maize was grown under axenic conditions and supplied with FeHMA, Fe uptake rates were 100-300 times higher compared to those in plants supplied with Fe siderophores. Fe from both sources was taken up without the involvement of an extracellular reduction process. The supply of FeHMA enhanced both uptake rate and translocation rate to the shoot (>60% of the total uptake). However, increased d. of microorganisms resulted in a decrease in Fe uptake rate (up to 65%), presumably due to microbial degradation of the FeHMA. In contrast, when FeFOB or FePSB was used as the Fe source, increased population d. of microorganisms enhanced Fe uptake. The enhancement of Fe uptake resulted from the uptake of FeFOB and FePSB by microorganisms adhering to the rhizoplane or living in the free space of cortical cells. The microbial apoplastic Fe pool was not available for root to shoot transport or, thus, for utilization by the plants. These results, in addition to the low uptake rate under axenic conditions, are in contrast to earlier hypotheses suggesting the existence of a specific uptake system for Fe siderophores in higher plants. The bacterial siderophores PSB and FOB were inefficient as Fe sources for plants even when supplied by stem injection. It was concluded that microorganisms are involved in degradation processes of microbial siderophores, as well as in competition for Fe with higher plants.

IT 76975-04-7, Pseudobactin

RL: BIOL (Biological study)

(iron uptake by corn and oat in response to rhizospheric microorganisms in relation to)

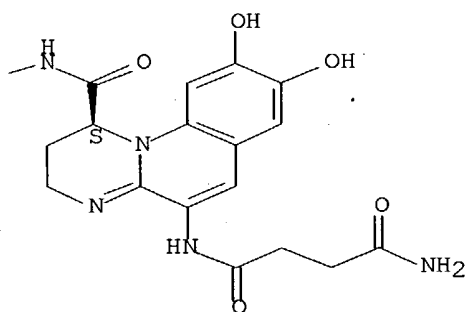
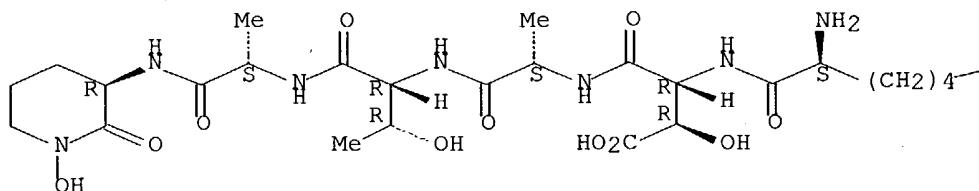
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

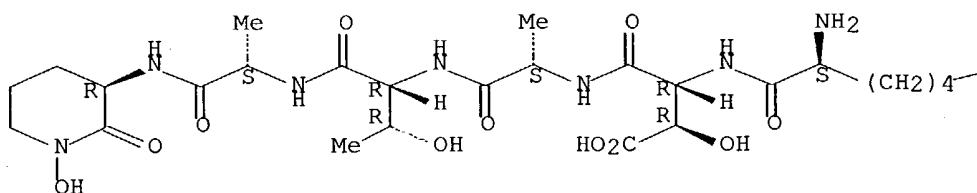
D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

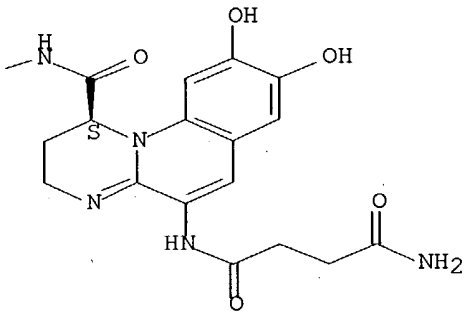


IT 76975-04-7D, iron complexes
 RL: BIOL (Biological study)
 (iron uptake by corn and oat response to rhizospheric microorganisms
 in relation to)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-
 D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-B



L14 ANSWER 60 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1992:648390 CAPLUS Full-text

DN 117:248390

TI Utilization of the siderophores FOB and pseudobactin by rhizosphere microorganisms of cotton plants

AU Jurkevitch, Edouard; Hadar, Yitzhak; Chen, Yona

CS Fac. Agric., Hebrew Univ. Jerusalem, Rehovot, 76100, Israel

SO Journal of Plant Nutrition (1992), 15(10), 2183-92

CODEN: JPNUDS; ISSN: 0190-4167

DT Journal

LA English

AB The hydroxamate siderophores ferrioxamine B (FOB) and the pseudobactin siderophores st3 (PSBst3) and 7NSK2 (PSB7nsk2) were evaluated as iron (Fe) sources to cotton (*Gossypium herbeceum*) rhizosphere bacteria. About 13% of the total bacterial CFUs were able to utilize FeFOB as the sole Fe source in an Fe-deficient medium, as compared to 1.6 and 2.6% being able to utilize the chelated Fe supplied as Fe-pseudobactins St3 and 7NSK2, resp. Cotton plants grown in soil amended with 55Fe-EDDHA had about ten times more Fe in their leaves than when supplied with 55Fe-PSBst3. In a treatment in which the cells of strain 3 (St3) were added to the soil, about twice as much radioactivity was associated with the roots (on a gram fresh weight basis) of plants irrigated with PSBst3 than in the non-inoculated control treatment. These data suggest that pseudobactin is intrinsically a less available source of Fe to microbes than FOB and that the composition of the bacterial population of the rhizosphere may play an important role in transport and mobilization of Fe in this environment.

IT 76975-04-7, Pseudobactin

RL: BIOL (Biological study)

(utilization of iron of, by cotton rhizosphere bacteria)

RN 76975-04-7 CAPLUS

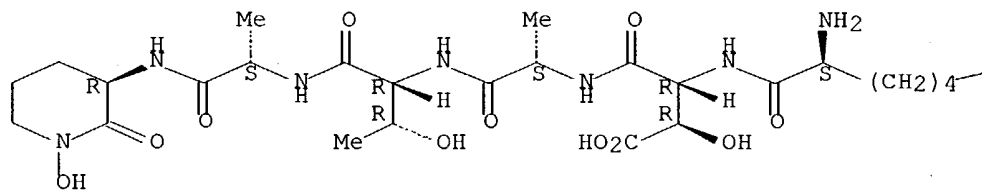
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

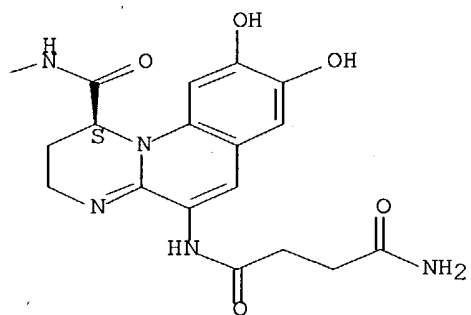
dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





L14 ANSWER 61 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1992:565454 CAPLUS Full-text

DN 117:165454

TI Inhibition of iron overload toxicity in rat hepatocyte cultures by desferrioxamine B and pyoverdin Pf, the siderophore of *Pseudomonas fluorescens*

AU Jago, Patrick; Hubert, Noella; Morel, Isabelle; Pasdeloup, Nicole; Okactan, Aydin Z.; Abdallah, Mohamed; Brissot, Pierre; Lescoat, Gerard

CS Unite Rech. Hepatol., INSERM, Rennes, 35033, Fr.

SO Colloque INSERM (1992), 216(Cell Mol. Aspects Cirrhosis), 85-8

CODEN: CINMDE; ISSN: 0768-3154

DT Journal

LA English

AB Iron overload was toxic for adult rat hepatocyte cultures since the release of LDH in the culture medium was increased whereas its intracellular level was decreased. This toxicity was also confirmed by a decrease in albumin secretion and an increase in total free malondialdehyde production. The toxic effect of iron overload in rat hepatocyte cultures was inhibited by desferrioxamine B. Pyoverdin Pf was as effective as desferrioxamine B in the protection of hepatocyte cultures against this toxic effect. The mechanisms by which desferrioxamine B and pyoverdin Pf may act are related to their powerful ability to chelate iron.

IT **130145-73-2**, Pyoverdin Pf

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological

study, unclassified); BIOL (Biological study)

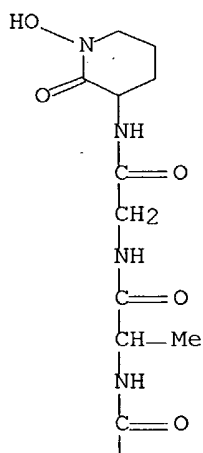
(iron toxicity to hepatocytes response to)

RN 130145-73-2 CAPLUS

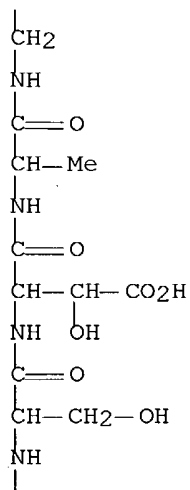
CN Glycinamide, N-[[[2-[1-[[[5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-2,3-

dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]amino]-2-hydroxyethyl]-1,4,5,6-tetrahydro-5-pyrimidinyl]carbonyl]glycyl-L-seryl-threo-3-hydroxy-D- α -aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, conjugate monoacid (9CI) (CA INDEX NAME)

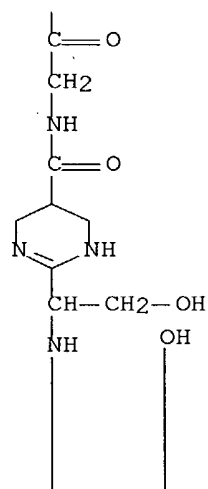
PAGE 1-A



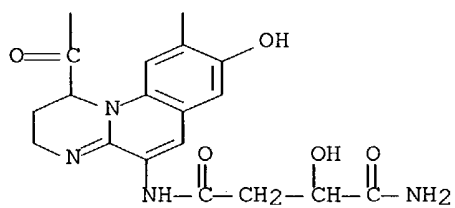
PAGE 2-A



PAGE 3-A



PAGE 4-A



● H⁺

L14 ANSWER 62 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1992:443972 CAPLUS Full-text

DN 117:43972

TI Isolation and characterization of pseudobactin B: a pseudobactin-type siderophore from *Pseudomonas* species strain PD 30

AU Andriollo, Nunzio; Guarini, Alessandro; Cassani, Giorgio

CS Ist. Guido Donegani S.p.A., ENICHEM, Novara, 28100, Italy

SO Journal of Agricultural and Food Chemistry (1992), 40(7), 1245-8

CODEN: JAFCAU; ISSN: 0021-8561

DT Journal

LA English

AB A simple method is discussed for the isolation of pseudobactin B, a new siderophore produced together with pseudobactin by plant growth promoting bacterium *Pseudomonas* PD 30. Pseudobactin B differs from the known pseudobactin only by the nature of the dicarboxylic acid attached to the chromophore, which is succinic acid instead of succinamide. The structure of pseudobactin B was determined by a comparison of its ¹H NMR, UV, and mass spectra with those of pseudobactin. An HPLC assay for pseudobactin B and pseudobactin, quantification in fermentation beer, and a new efficient method for isolating them are proposed.

IT 76975-04-7, Pseudobactin

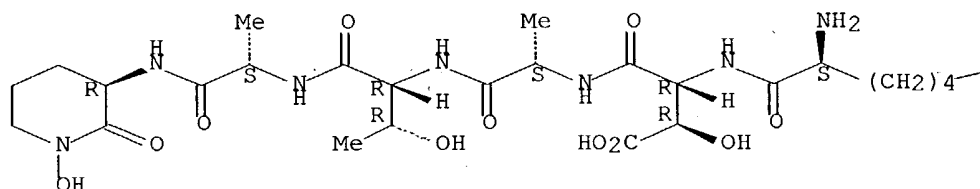
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by HPLC)

RN 76975-04-7 CAPLUS

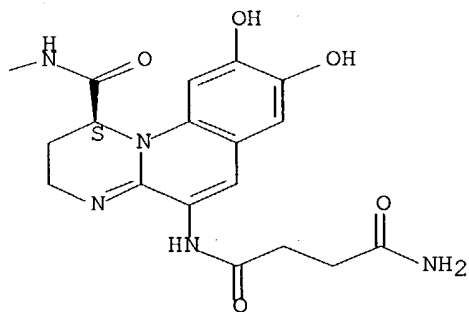
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B



IT 138145-39-8

RL: ANST (Analytical study)

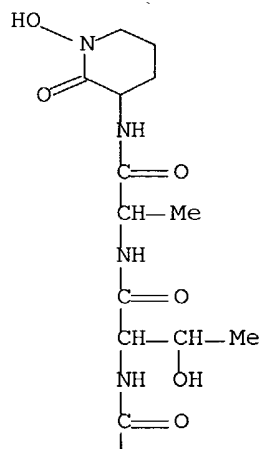
(from *Pseudomonas*, isolation and characterization of)

RN 138145-39-8 CAPLUS

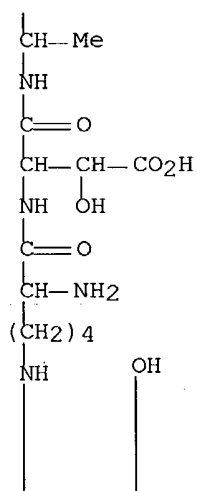
CN L-Alaninamide, N6-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro

8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3S)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

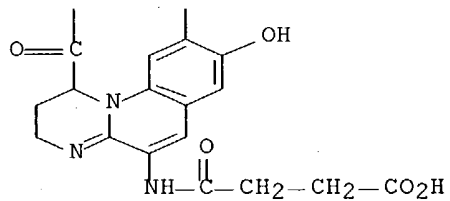
PAGE 1-A



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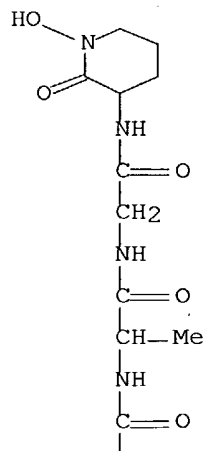


PAGE 3-A

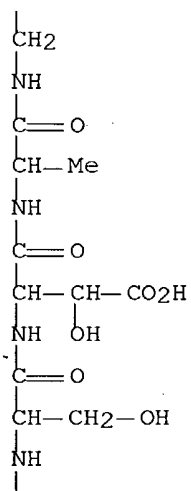


L14 ANSWER 63 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1992:229784 CAPLUS Full-text
 DN 116:229784
 TI Inhibition of iron overload toxicity in rat hepatocyte cultures by
 pyoverdin Pf, the siderophore of *Pseudomonas fluorescens*
 AU Jegu, Patrick; Hubert, Noella; Morel, Isabelle; Pasdeloup, Nicole;
 Ocaktan, Aydin; Abdallah, Mohamed; Brissot, Pierre; Lescoat, Gerard
 CS Liver Res. Unit, Pontchaillou Univ., Rennes, 35033, Fr.
 SO Biochemical Pharmacology (1992), 43(6), 1275-80
 CODEN: BCPA6; ISSN: 0006-2952
 DT Journal
 LA English
 AB The effect of the pyoverdin Pf (an iron chelating agent isolated and
 purified from *P. fluorescens* CCM 2798) was studied on iron-overloaded
 rat hepatocyte cultures. Iron overload was obtained by addition of 5-80
 μ M ferric nitrilotriacetate to the culture medium. Twenty-four hours
 after iron treatment, a significant increase in aspartate
 aminotransferase and lactate dehydrogenase in the culture medium was
 observed. This corresponded to an intracellular decrease in the activity
 of these two enzymes and correlated with a decrease in albumin secretion
 and an increase in total free malondialdehyde production. The iron
 toxicity was inhibited by desferrioxamine B. Pyoverdin Pf added to the
 hepatocyte cultures served as an effective agent to prevent iron
 toxicity induced in overload. The observed effect of the pyoverdin Pf
 was as potent as that of desferrioxamine B.
 IT **130145-73-2**
 RL: BIOL (Biological study)
 (iron toxicity to hepatocytes inhibition by)
 RN 130145-73-2 CAPLUS
 CN Glycinamide, N-[[[2-[1-[[[5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-
 2,3-
 dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]amino]-2-
 hydroxyethyl]-1,4,5,6-tetrahydro-5-pyrimidinyl]carbonyl]glycyl-L-seryl-
 threo-3-hydroxy-D- α -aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-
 oxo-3-piperidinyl)-, conjugate monoacid (9CI) (CA INDEX NAME)

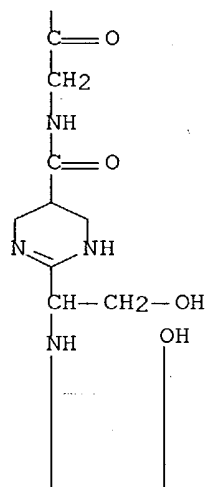
PAGE 1-A



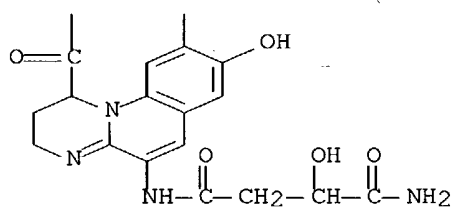
PAGE 2-A



PAGE 3-A



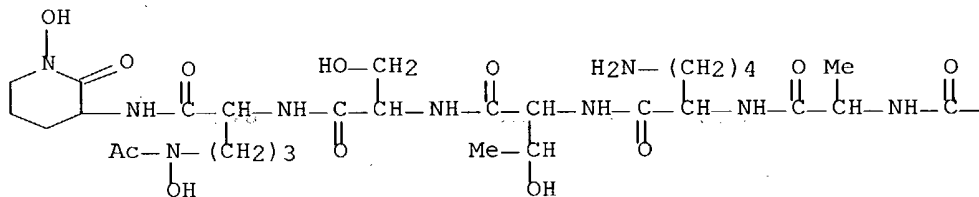
PAGE 4-A



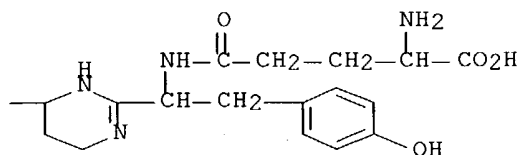
● H⁺

L14 ANSWER 64 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1992:169760 CAPLUS Full-text
 DN 116:169760
 TI Bacterial components. The biogenesis of Pseudomonas siderophores: the proof of analogous structures of a pyoverdin/desferri-ferribactin pair
 AU Budzikiewicz, H.; Schroeder, H.; Taraz, K.
 CS Inst. Org. Chem., Univ. Koeln, Cologne, D-5000/41, Germany
 SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1992), 47(1-2), 26-32
 CODEN: ZNCBDA; ISSN: 0341-0382
 DT Journal
 LA German
 AB When grown in an iron-deficient medium, Pseudomonas aptata produces both a desferri-ferribactin and a pyoverdin. The identical sequence of the peptide chain confirms the hypothesis that desferri-ferribactins are the biogenetic precursors of pyoverdins.
 IT **140198-04-5 140198-05-6**
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
 (of Pseudomonas aptata)
 RN 140198-04-5 CAPLUS
 CN L-Ornithinamide, N-[[2-[1-[(4-amino-4-carboxy-1-oxobutyl)amino]-2-(4-hydroxyphenyl)ethyl]-1,4,5,6-tetrahydro-4-pyrimidinyl]carbonyl]-D-alanyl-L-lysyl-L-threonyl-D-seryl-N5-acetyl-N5-hydroxy-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1[4S-[2[S*(R*)],4R*]],5(S)]- (9CI) (CA INDEX NAME)

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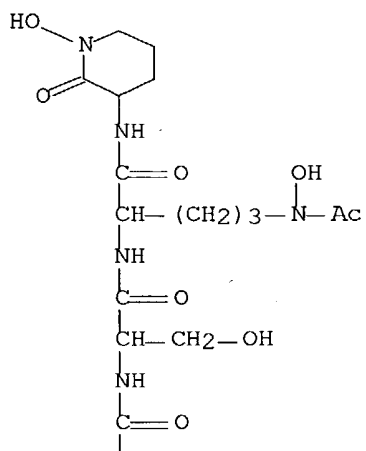
PAGE 1-B



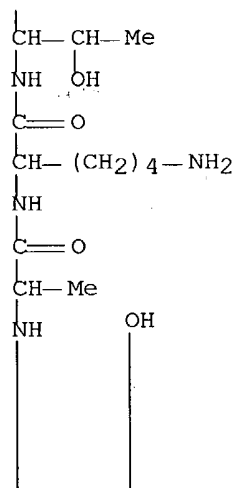
RN 140198-05-6 CAPLUS
 CN L-Ornithinamide, N-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-L-lysyl-L-threonyl-D-seryl-N5-acetyl-N5-hydroxy-N-(1-hydroxy-2-oxo-3-piperidinyl)-

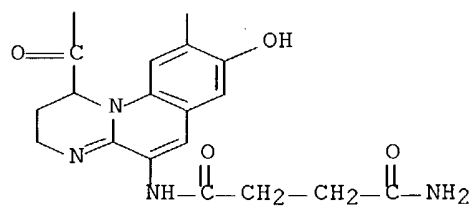
[1(S),5(S)]- (9CI) (CA INDEX NAME)

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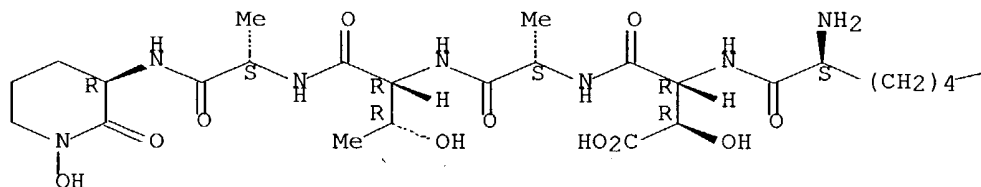


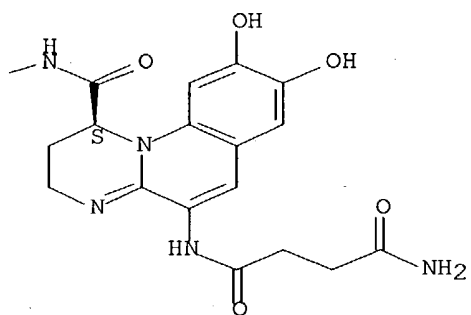


L14 ANSWER 65 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1992:37835 CAPLUS Full-text
 DN 116:37835
 TI Effects of iron(III) analogs on growth and isolate
 AU Fekete, Frank A.; Barton, Larry L.
 CS Dep. Biol., Univ. New Mexico, Albuquerque, NM, 87131-1091, USA
 SO Biology of Metals (1991), 4(4), 211-16
 CODEN: BMETE8; ISSN: 0933-5854
 DT Journal
 LA English
 AB The growth and siderophore production of a fluorescent *Pseudomonas* species isolated from soil contaminated with Cr was influenced by the presence of trivalent cations. Overprod. of pseudobactin occurred when the isolate was grown in media containing 1 mM Cr(III) under Fe-limited conditions but not when Fe(III) was added at 10 μ M. Pseudobactin synthesis was derepressed in Fe-limited cultures containing 1 mM Sc(III) or Y(III), examples of group III-B elements. Al(III), Ga(III) or In(III), representative metals from group III-A, repressed synthesis of pseudobactin under Fe-deficient conditions. Analogs of Fe(III) inhibited the *Pseudomonas* isolate in iron-limited media and the trivalent metals listed in order of decreasing toxicity were as follows: Ga > In > Sc > Cr > Y > Al. The inhibition of growth by 1 mM In(III), Sc(III), and Ga(III) was greater during Fe-limited growth than in media containing 10 μ M Fe(III). Although the metal analogs of Fe(III) have similar chemical and phys. characteristics, the physiol. response of the fluorescent pseudomonad when grown in the presence of these metals varied markedly.
 IT **76975-04-7**, Pseudobactin
 RL: FORM (Formation, nonpreparative)
 (formation of, by *Pseudomonas*, iron analogs effect on)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

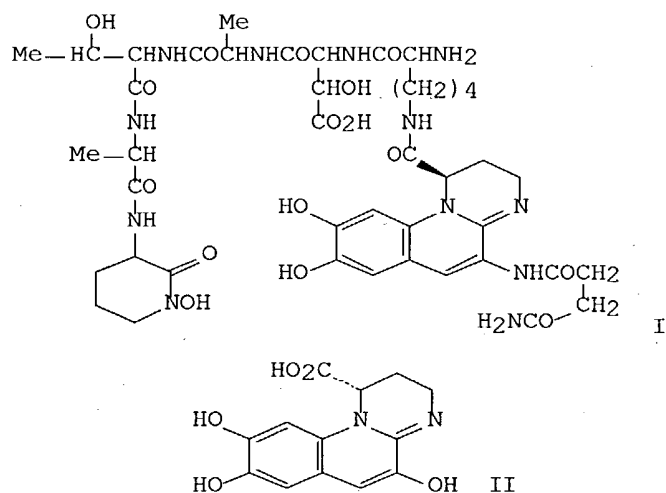
Absolute stereochemistry.

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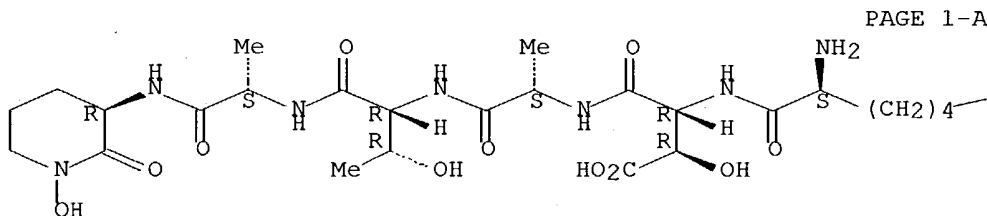


L14 ANSWER 66 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1992:18115 CAPLUS Full-text
 DN 116:18115
 TI Variants of pseudobactin and pseudobactin A: new pyoverdin type peptide siderophores from *Pseudomonas fluorescens* "E2"
 AU Taraz, K.; Seinsche, D.; Budzikiewicz, H.
 CS Inst. Org. Chem., Univ. Cologne, Cologne, D-5000/41, Germany
 SO Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1991), 46(7-8), 522-6
 CODEN: ZNCBDA; ISSN: 0341-0382
 DT Journal
 LA German
 GI

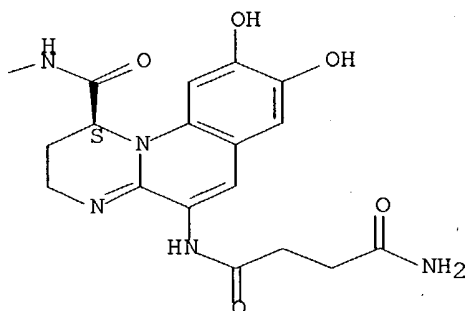


AB Pseudobactin (I) and several related compds. were isolated from a strain of *P. fluorescens* and their structures were elucidated. In this way a reference compound (II) could be obtained for the unambiguous determination of the absolute configuration of C-1 of the pyoverdin chromophore in newly isolated representatives of this class.
 IT **76975-04-7**, Pseudobactin
 RL: PRP (Properties) (configuration of)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



PAGE 1-A



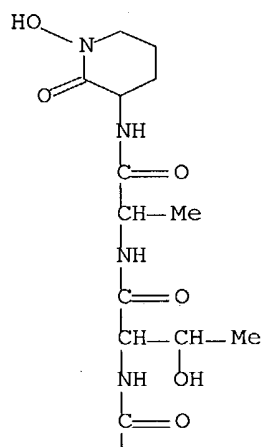
IT 138145-39-8 138145-40-1 138145-41-2

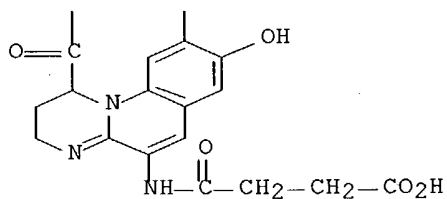
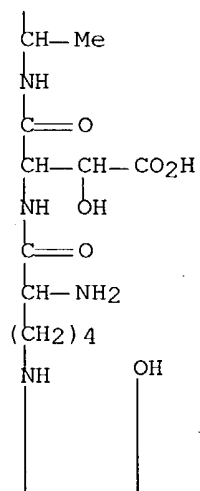
RL: BIOL (Biological study)

(peptide siderophore, of *Pseudomonas fluorescens*)

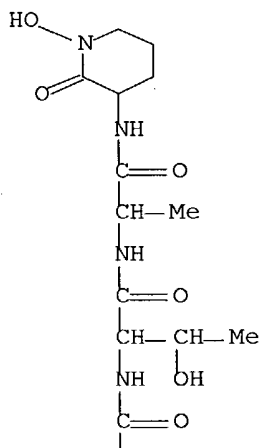
RN 138145-39-8 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3S)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

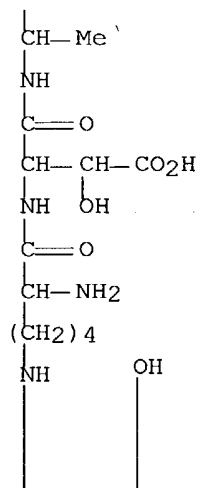




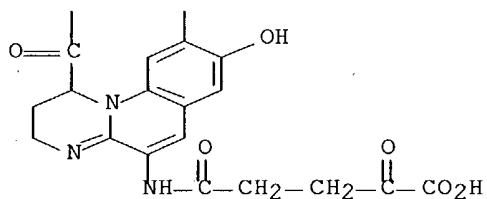
RN 138145-40-1 CAPLUS
 CN L-Alaninamide, N6-[[5-[(4-carboxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-threo-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1(S),5(R)]- (9CI) (CA INDEX NAME)



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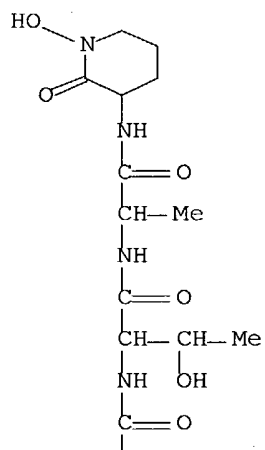


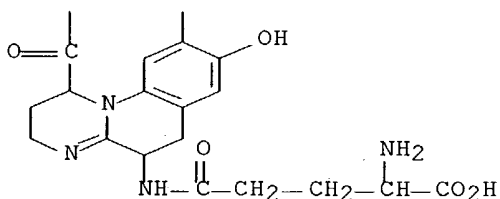
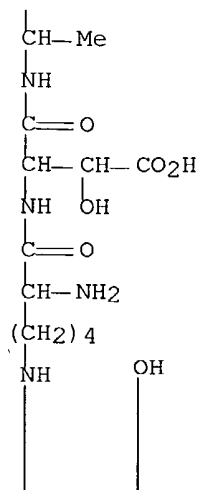
PAGE 3-A



RN 138145-41-2 CAPLUS
 CN L-Alaninamide, N6-[[5-[(4-amino-4-carboxy-1-oxobutyl)amino]-2,3,5,6-tetrahydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3S)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

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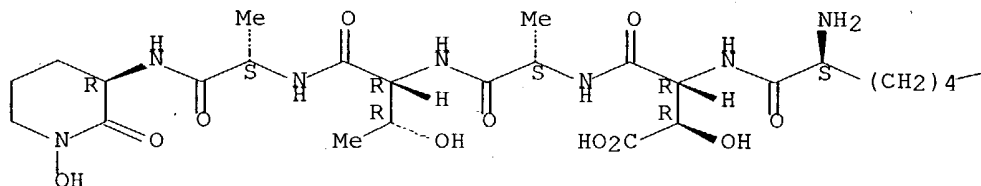


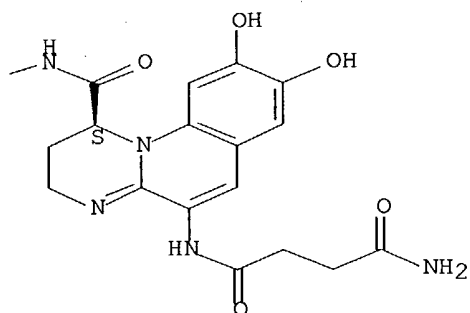
IT 76975-04-7DP, iron complex 138145-39-8DP, iron complex
 138145-40-1DP, iron complex 138145-41-2DP, iron complex
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 76975-04-7 CAPLUS

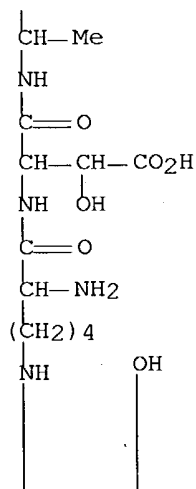
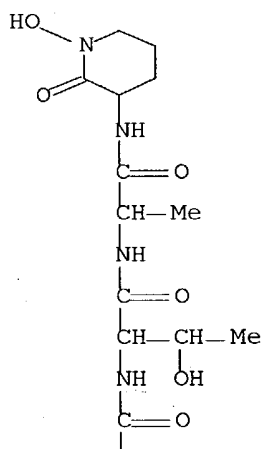
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

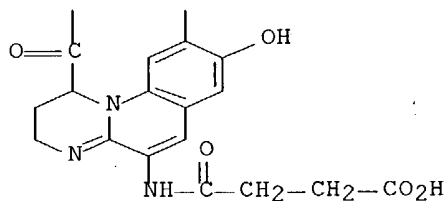
Absolute stereochemistry.



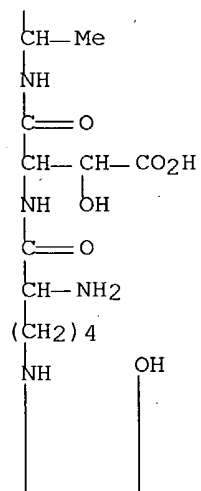
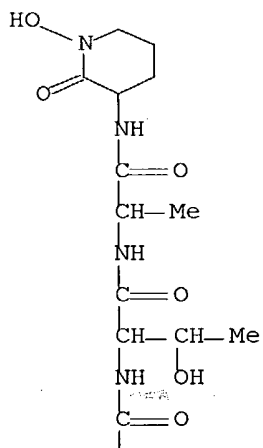


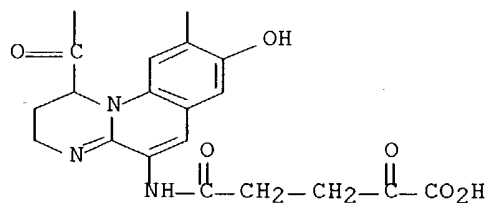
RN 138145-39-8 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3S)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)



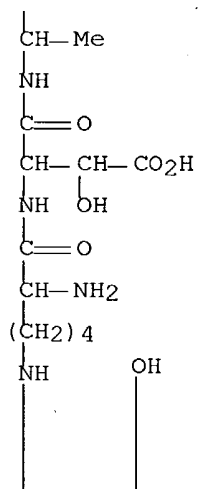
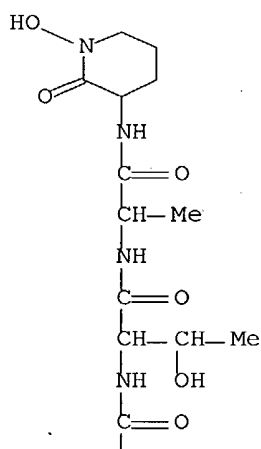


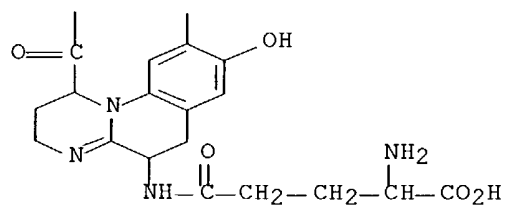
RN	138145-40-1	CAPLUS
CN	L-Alaninamide, N6-[[5-[(4-carboxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-threo-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1(S),5(R)]- (9CI) (CA INDEX NAME)	





RN 138145-41-2 CAPLUS
 CN L-Alaninamide, N6-[[5-[(4-amino-4-carboxy-1-oxobutyl)amino]-2,3,5,6-tetrahydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3S)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidiny)- (9CI) (CA INDEX NAME)





L14 ANSWER 67 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:181626 CAPLUS Full-text

DN 114:181626

TI Development of a detection system for ferric pseudobactin using monoclonal

antibodies

AU Buyer, J. S.; Sikora, L. J.; Kratzke, M. G.

CS Soil Microb. Syst. Lab., NRI, Beltsville, MD, 20705, USA

SO Plant and Soil (1991), 130(1-2), 243-7

CODEN: PLSOA2; ISSN: 0032-079X

DT Journal

LA English

AB Monoclonal antibodies (MAbs) were produced to ferric pseudobactin, the siderophore of plant growth-promoting *Pseudomonas* B10. Three IgG1 MAbs cross-react with certain ferric pseudobactins but not with others. A competitive ELISA was developed to detect and quantify ferric pseudobactin.

IT **76975-04-7D**, complexes with iron

RL: ANT (Analyte); ANST (Analytical study)

(determination of, by ELISA, monoclonal antibodies for)

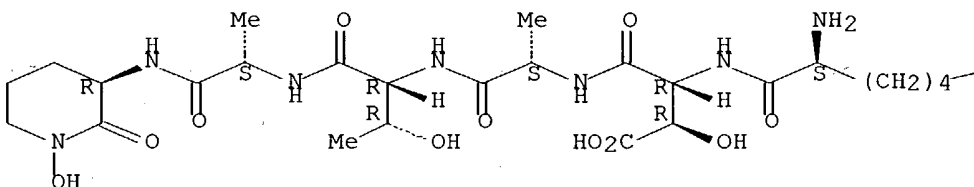
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

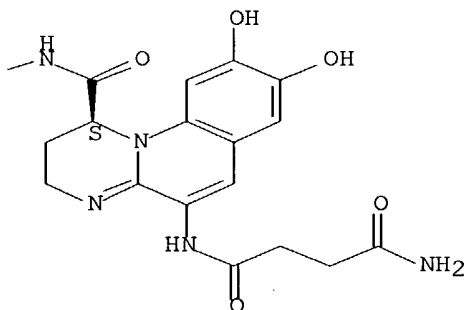
D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

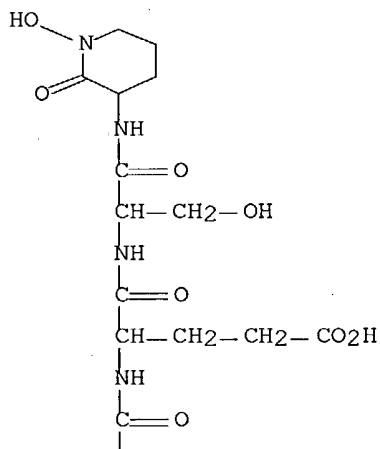


PAGE 1-B

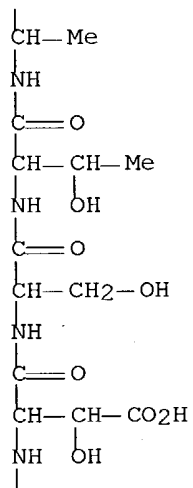


L14 ANSWER 68 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1991:180627 CAPLUS Full-text
 DN 114:180627
 TI Purification, characterization, and structure of pseudobactin 589 A, a siderophore from a plant growth promoting *Pseudomonas* [Erratum to document cited in CA113(9):73258b]
 AU Persmark, Magnus; Frejd, Torbjoern; Mattiasson, Bo
 CS Chem. Cent., Univ. Lund, Lund, S-221 00, Swed.
 SO Biochemistry (1991), 30(7), 2010
 CODEN: BICHAW; ISSN: 0006-2960
 DT Journal
 LA English
 AB An error in Figure 1A has been corrected The error was not reflected in the abstract or the index entries.
 IT **128023-08-5P**
 RL: PREP (Preparation)
 (of *Pseudomonas putida*, purification and characterization and structure of (Erratum))
 RN 128023-08-5 CAPLUS
 CN Serinamide, N6-[N-[[5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L- α -aspartyl]-L-lysyl-threo-3-hydroxy-D- α -aspartylseryl-L-threonyl-D-alanyl-D- α -glutamyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1[S-(R*,R*)],7(S)]- (9CI) (CA INDEX NAME)

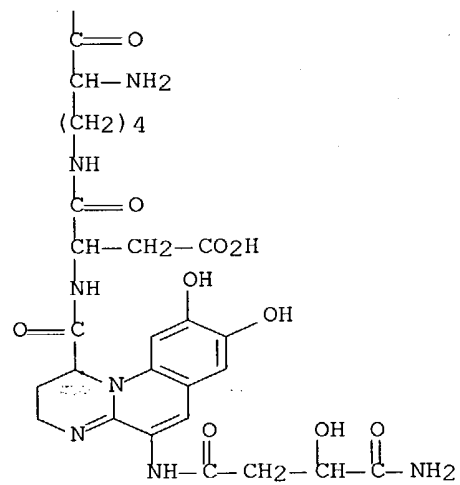
PAGE 1-A



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AN 1991:142196 CAPLUS Full-text

DN 114:142196

TI Siderophores of *Pseudomonas putida* as an iron source for dicot and monocot

plants

AU Bar-Ness, E.; Chen, Y.; Hadar, Y.; Marschner, H.; Roemheld, V.

CS Fac. Agric., Hebrew Univ. Jerusalem, Rehovot, 76100, Israel

SO Plant and Soil (1991), 130(1-2), 231-41

CODEN: PLSOA2; ISSN: 0032-079X

DT Journal

LA English

AB Iron uptake from ferrated (^{59}Fe) pseudobactin (PSB), a *P. putida* siderophore, by various plant species was studied in nutrient solution culture under short-term (10 h) and long-term (3 wk) conditions. In the short-term expts., ^{59}Fe uptake rate from $^{59}\text{FePSB}$ by dicots (peanuts, cotton and sunflower) was relatively low when compared with ^{59}Fe uptake rate from $^{59}\text{FeEDDHA}$. Iron uptake rate from $^{59}\text{FePSB}$ was pH and concentration dependent, as was the Fe uptake rate from $^{59}\text{FeEDDHA}$. The rate was about 10 times lower than that of Fe uptake from the synthetic chelate. Results were similar for long-term expts. Monocots (sorghum) in short-term expts. exhibited significantly higher uptake rate of Fe from $^{59}\text{FePSB}$ than from $^{59}\text{FeEDDHA}$. In long-term expts., $^{59}\text{FePSB}$ was less efficient than $^{59}\text{FeEDDHA}$ as an Fe source for sorghum at pH 6, but the same levels of leaf chlorophyll concentration were obtained at pH 7.3. Fe uptake rates by dicots from the siderophore and $^{59}\text{FeEDDHA}$ were found to correlate with Fe reduction rates and reduction potentials (E_0) of both chelates. Therefore, it is suggested that the reduction mechanism governs the Fe uptake process from PSB by dicots.

IT **76975-04-7D**, Pseudobactin, ferrated

RL: BIOL (Biological study)

(iron uptake from, by monocotyledonous and dicotyledonous plants)

RN 76975-04-7 CAPLUS

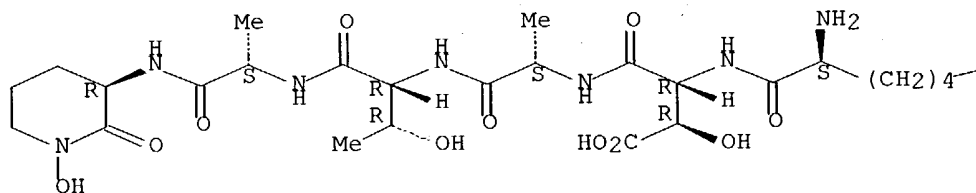
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

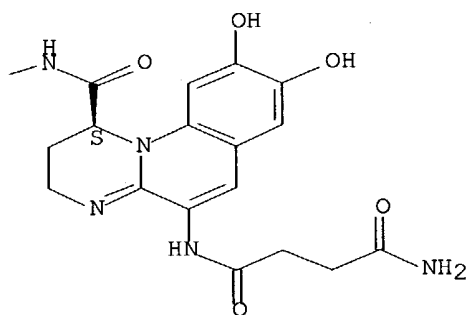
dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

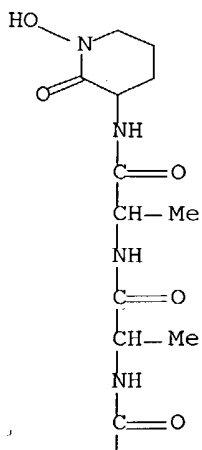
PAGE 1-A



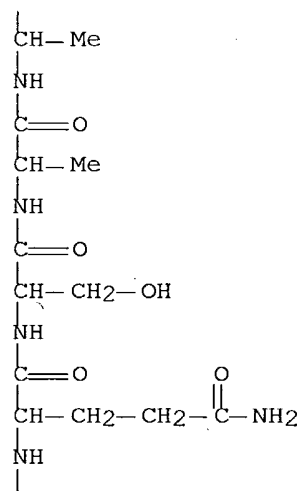


L14 ANSWER 70 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1991:58570 CAPLUS Full-text
 DN 114:58570
 TI Bacterial constituents. XLII. New pyoverdin-type siderophores from *Pseudomonas fluorescens*
 AU Mohn, G.; Taraz, K.; Budzikiewicz, H.
 CS Inst. Org. Chem., Cologne, D-5000/41, Germany
 SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1990), 45(10), 1437-50
 CODEN: ZNBSEN; ISSN: 0932-0776
 DT Journal
 LA English
 AB The structures of two new pyoverdins (GM-I and GM-II) isolated from the culture medium of *Pseudomonas fluorescens* have been elucidated by spectroscopic methods and degradation studies. The pyoverdins consist of a chromophore which could be identified as (1S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinoline-1-carboxylic acid substituted at the amino group with a 3-carboxypropanoyl or a succinamoyl residue and at the carboxy group with the N-terminus of D-Ala-D-Lys-Gly-Gly-D-threo-(OH)Asp-D-Glu-D-Ser-D-Ala-D-Ala-D-Ala-L-Ala-L-N5-(OH)Orn. According to the "short-hand" nomenclature proposed the two compds. should be characterized as pyoverdin-Q-akGGd'qsAaaAO'*-SUCA and pyoverdin-Q-akGGd'qsAaaAO'*-SUC.
 IT **131647-39-7, GM-I 131647-40-0, GM-II**
 RL: BIOL (Biological study)
 (from *Pseudomonas fluorescens*)
 RN 131647-39-7 CAPLUS
 CN L-Alaninamide, N-[[5-(4-amino-1,4-dioxobutyl)-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-L-lysylglycylglycyl-threo-3-hydroxy-D- α -aspartyl-D-glutaminy-D-seryl-L-alanyl-D-alanyl-D-alanyl-N-(1-hydroxy-2-oxo-3-piperidiny)- (9CI) (CA INDEX NAME)

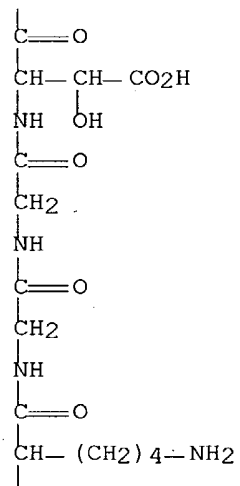
PAGE 1-A

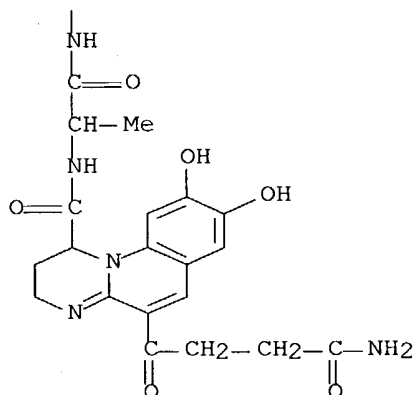


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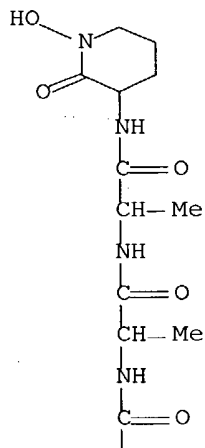


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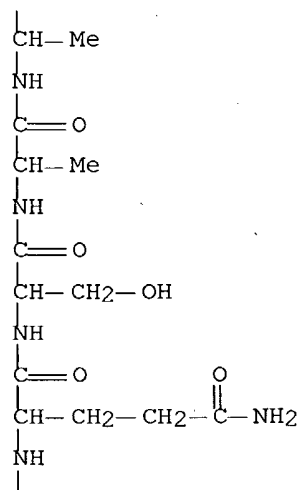




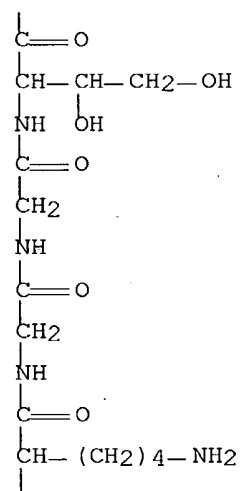
RN 131647-40-0 CAPLUS
 CN L-Alaninamide, N-[[5-(4-amino-1,4-dioxobutyl)-2,3-dihydro-8,9-dihydroxy-
 1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-alanyl-L-lysylglycylglycyl-4-
 hydroxy-D-threonyl-D-glutaminy-D-seryl-L-alanyl-D-alanyl-D-alanyl-N-(1-
 hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

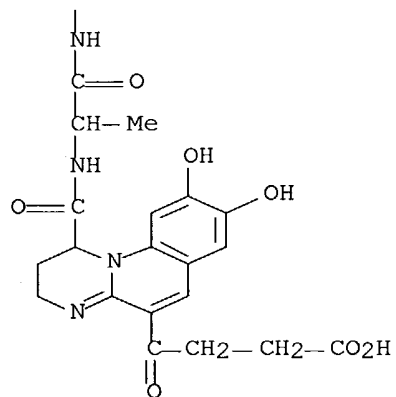


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L14 ANSWER 71 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:626590 CAPLUS Full-text

DN 113:226590

TI Bacterial siderophores: structures of pyoverdins Pt, siderophores of *Pseudomonas tolaasii* NCPPB 2192, and pyoverdins Pf, siderophores of *Pseudomonas fluorescens* CCM 2798. Identification of an unusual natural amino acid

AU Demange, Pascal; Bateman, Andrew; Mertz, Christian; Dell, Anne; Piemont, Yves; Abdallah, Mohamed A.

CS Dep. Chim., Univ. Louis Pasteur, Strasbourg, 67008, Fr.

SO Biochemistry (1990), 29(50), 11041-51

CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

AB Pyoverdins were isolated and characterized resp. from the cultures of *Pseudomonas tolaasii* NCPPB 2192 (pyoverdins Pt, Pt A, and Pt B) and *Pseudomonas fluorescens* CCM 2798 (pyoverdins Pf/1, Pf/2, Pf, Pf/3/1, and Pf/3/2) each grown in Fe-deficient conditions. Their structures were established by using FAB-MS, NMR, and CD techniques. These siderophores are chromopeptides, and all but one (pyoverdin Pf/3/3) possess at the N terminus of their peptide chain the same chromophore that has been reported in pyoverdin Pa from *Pseudomonas aeruginosa* ATCC 15692 and pseudobactin B 10 from *Pseudomonas* B10 which is derived from 2,3-diamino-6,7-dihydroxyquonoline. In pyoverdins Pt this chromophore is bound to a linear peptide chain D-Ser-L-Lys-D-Ser-L-Ser-L-Thr-D-Ser-L-OHOrn-L-Thr-D-Ser-D-OHOrn(cyclic) which has its C-terminal end blocked by cyclic D-N δ -hydroxyornithine. In pyoverdins Pf, the peptide chain is also linear, SerCTHPMD-Gly-L-Ser-D-threo-OHAsp-L-Ala-Gly-D-Ala-Gly-L-OHOrn(cyclic) (SerCTHPMD stands for 2-seryl-6-carboxy-3,4,5,6-tetrahydropyridine) and contains an unusual natural amino acid which is the result of the condensation of 1 mol of serine and 1 mol of 2,4-diaminobutyric acid, forming a cyclic amidine. The pyoverdins Pt differ only in a substituent bound to the N on C-3 of the chromophore, which is succinic acid in pyoverdin Pt A, succinamide in pyoverdin Pt, and α -ketoglutaric acid bound to the chromophore by its C-5 atom in pyoverdin Pt B. Similarly, pyoverdin Pf/1, pyoverdin Pf/2, pyoverdin Pf (the major compound), and pyoverdin Pf/3/2 are substituted resp. by L-malic acid, succinic acid, L-malic acid, and succinamide. Pyoverdin Pf/3/3 has the same chromophore as azotobactin, the peptidic siderophore of *Azotobacter vinelandii*. These pyoverdins are very similar to pseudobactin B 10, the siderophore of *Pseudomonas* B10: they are linear peptides containing three bidentate groups strongly chelating Fe(III) and blocked at their N-terminus by the catecholic chromophore and at their C terminus by cyclic N δ -hydroxyornithine. They differ therefore from other pyoverdins such as those from *P. aeruginosa* ATCC 15692 which contain a partly cyclic peptide.

IT 130145-73-2 130145-74-3 130145-75-4

130145-76-5 130167-82-7

RL: PRP (Properties)

(structure of, of *Pseudomonas fluorescens*)

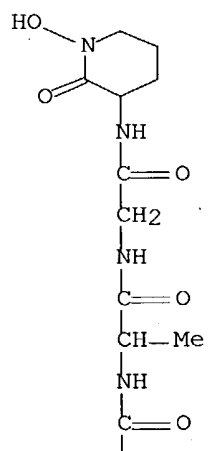
RN 130145-73-2 CAPLUS

CN Glycinamide, N-[[2-[1-[[[5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-2,3-

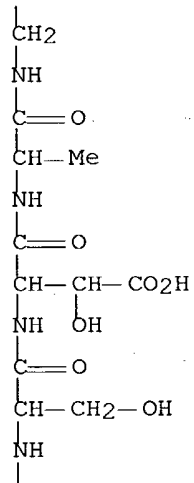
dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]amino]-2-hydroxyethyl]-1,4,5,6-tetrahydro-5-pyrimidinyl]carbonyl]glycyl-L-seryl-threo-3-hydroxy-D- α -aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-

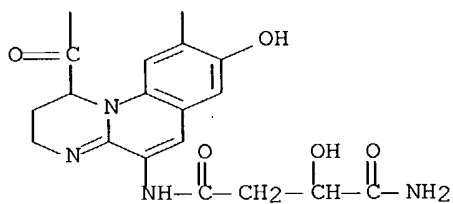
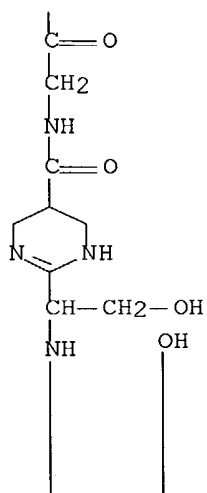
oxo-3-piperidinyl)-, conjugate monoacid (9CI) (CA INDEX NAME)

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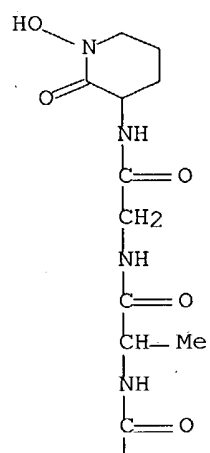
PAGE 2-A



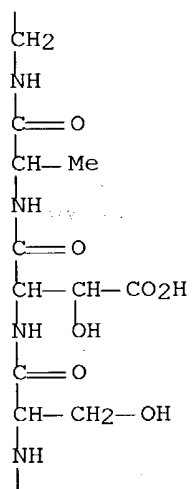


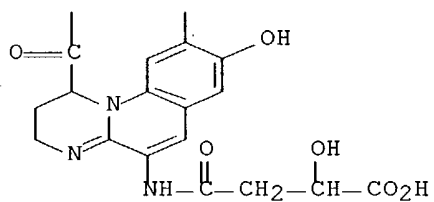
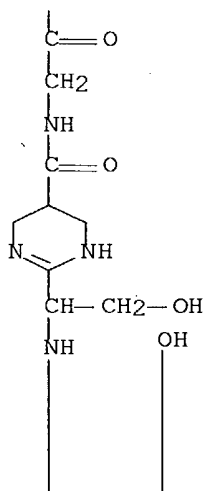
RN 130145-74-3 CAPLUS
 CN Glycinamide, N-[[2-[1-[[[5-[(3-carboxy-3-hydroxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]amino]-2-hydroxyethyl]-1,4,5,6-tetrahydro-5-pyrimidinyl]carbonyl]glycyl-L-seryl-threo-3-hydroxy-D-α-aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

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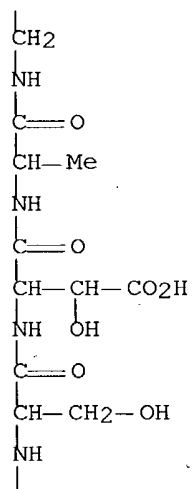
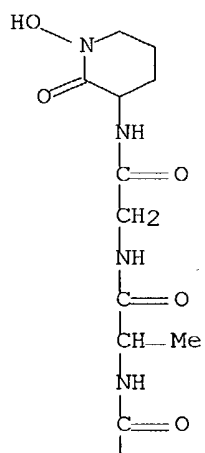


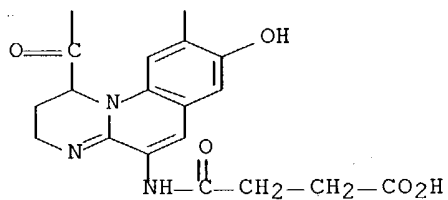
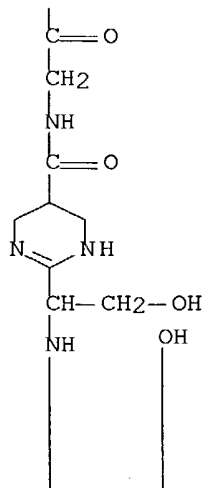
PAGE 2-A



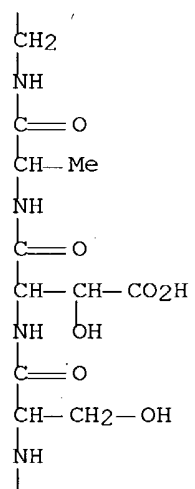
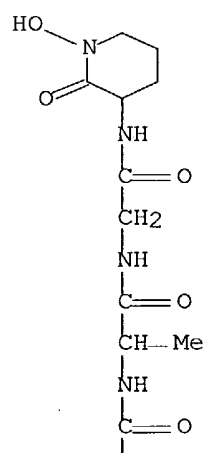


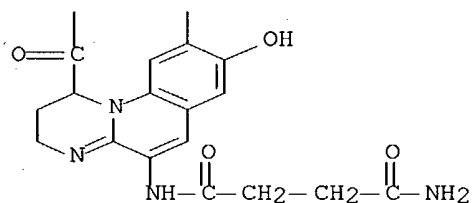
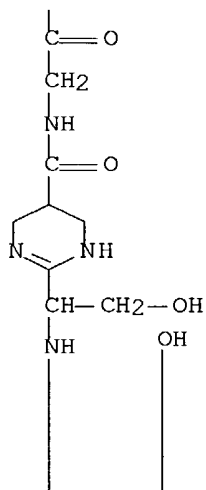
RN 130145-75-4 CAPLUS
 CN Glycinamide, N-[[2-[1-[[[5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]amino]-2-hydroxyethyl]-1,4,5,6-tetrahydro-5-pyrimidinyl]carbonyl]glycyl-L-seryl-threo-3-hydroxy-D- α -aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-(9CI) (CA INDEX NAME)



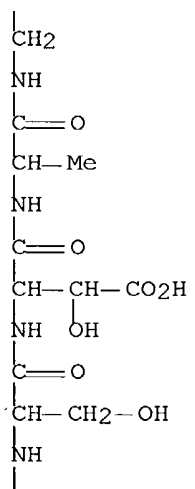
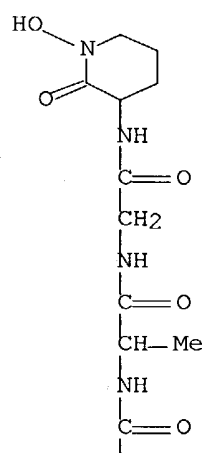


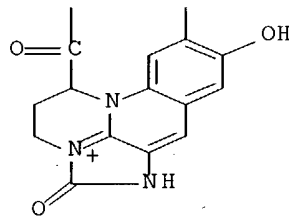
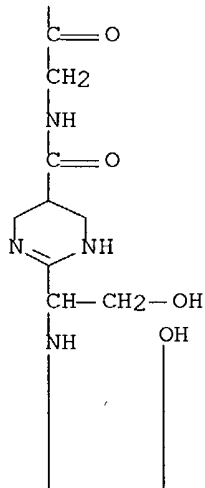
RN 130145-76-5 CAPLUS
 CN Glycinamide, N-[[2-[1-[[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]amino]-2-hydroxyethyl]-1,4,5,6-tetrahydro-5-pyrimidinyl]carbonyl]glycyl-L-seryl-threo-3-hydroxy-D- α -aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, conjugate monoacid (9CI) (CA INDEX NAME)





RN 130167-82-7 CAPLUS
 CN Glycinamide, N-[[[1,4,5,6-tetrahydro-2-[2-hydroxy-1-[[[2,3,4,5-tetrahydro-8,9-dihydroxy-4-oxo-1H-5,10b-diaza-3a-azoniaacephenanthrylen-1-yl)carbonyl]amino]ethyl]-5-pyrimidinyl]carbonyl]glycyl-L-seryl-threo-3-hydroxy-D-α-aspartyl-L-alanylglycyl-D-alanyl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)





IT 130145-72-1 130167-80-5 130167-81-6

RL: PRP (Properties)

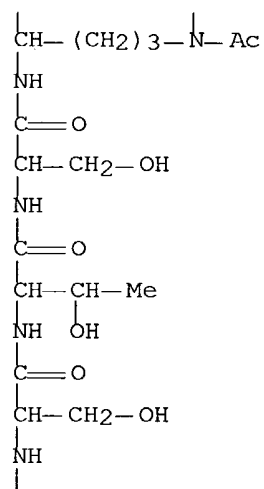
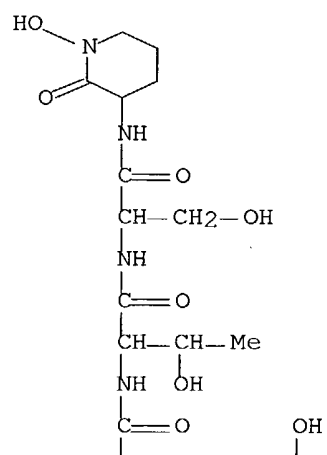
(structure of, of *Pseudomonas tolaasii*)

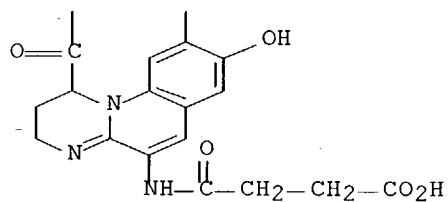
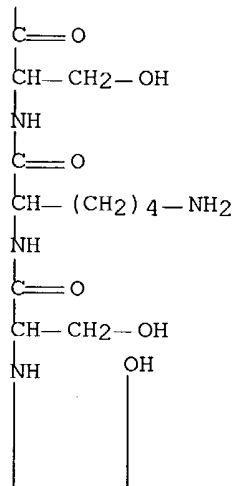
RN 130145-72-1 CAPLUS

CN D-Serinamide, N-[[5-[(3-carboxy-1-oxopropyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-L-seryl-D-seryl-L-threonyl-D-seryl-N5-acetyl-N5-hydroxy-L-ornithyl-L-threonyl-N-(1-hydroxy-2-oxo-3-piperidiny)-, [1(S),9(R)]- (9CI) (CA

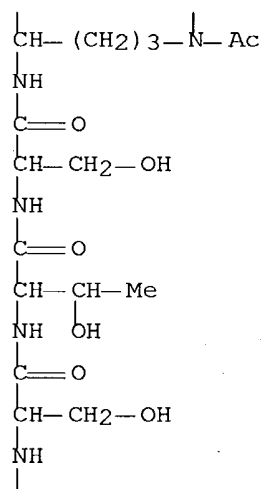
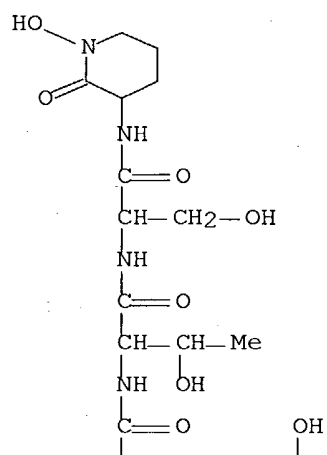
INDEX

NAME)

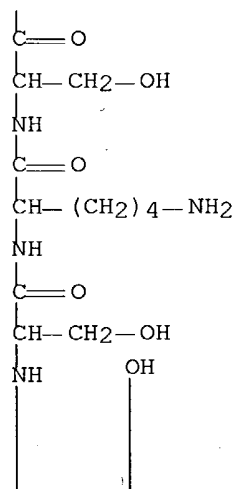




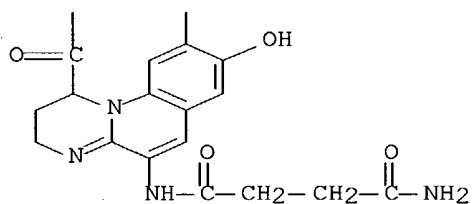
RN 130167-80-5 CAPLUS
 CN D-Serinamide, N-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-L-seryl-D-seryl-L-threonyl-D-seryl-N5-acetyl-N5-hydroxy-L-ornithyl-L-threonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, conjugate monoacid, [1(S),9(R)]- (9CI) (CA INDEX NAME)



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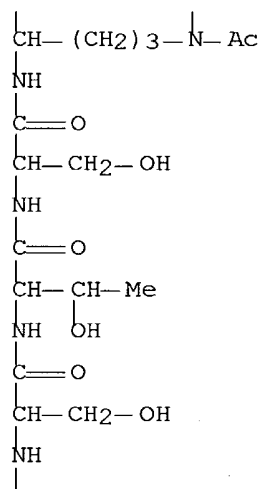
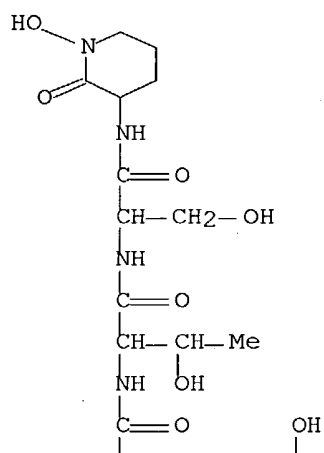


PAGE 4-A

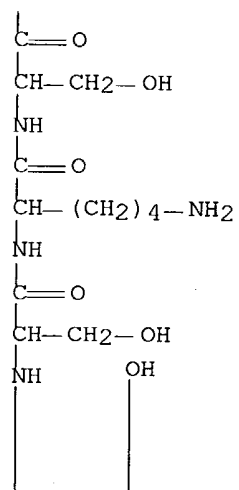


● H⁺

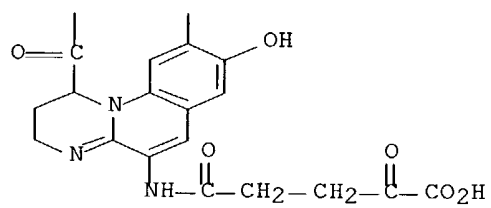
RN 130167-81-6 CAPLUS
 CN D-Serinamide, N-[[5-[(4-carboxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-D-seryl-L-lysyl-L-seryl-D-seryl-L-threonyl-D-seryl-N5-acetyl-N5-hydroxy-L-ornithyl-L-threonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1(S),9(R)]- (9CI) (CA
 INDEX
 NAME)



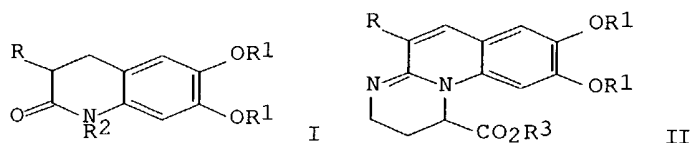
PAGE 3-A



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L14 ANSWER 72 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1990:477985 CAPLUS Full-text
 DN 113:77985
 TI Synthesis of the chromophore of pseudobactin, a fluorescent siderophore from *Pseudomonas*
 AU Kolasa, Teodozyj; Miller, Marvin J.
 CS Dep. Chem. Biochem., Univ. Notre Dame, Notre Dame, IN, 46556, USA
 SO Journal of Organic Chemistry (1990), 55(14), 4246-55
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 OS CASREACT 113:77985
 GI



AB Protected forms of dihydroxyphenylalanine were converted to the dihydroquinolinones I ($R = \text{NHCO}_2\text{CH}_2\text{CH}:\text{CH}_2$, phthalimido, succinimido; $R_1 = \text{CH}_2\text{Ph}$, Me; $R_2 = \text{H}$) by nitration and reductive cyclization. Subsequent N-alkylation with α -halo- γ -aminobutyric acid derivs. provided the carbon framework I ($R_2 = R_4\text{CH}_2\text{CH}_2\text{CHCO}_2R_3$, $R_3 = \text{CMe}_3$, Me, allyl; $R_4 = \text{NHCO}_2\text{CH}_2\text{CH}:\text{CH}_2$, phthalimido, $\text{NHCO}_2\text{CMe}_3$) for the chromophore of pseudobactin. Conversion to protected forms of the fluorescent chromophore II was accomplished by reaction of I ($R_2 = R_4\text{CH}_2\text{CH}_2\text{CHCO}_2R_3$) with Lawesson's reagent to produce the thioamide which was cyclized by reaction with $\text{Hg}(\text{OAc})_2$.

IT **76975-04-7P**, Pseudobactin

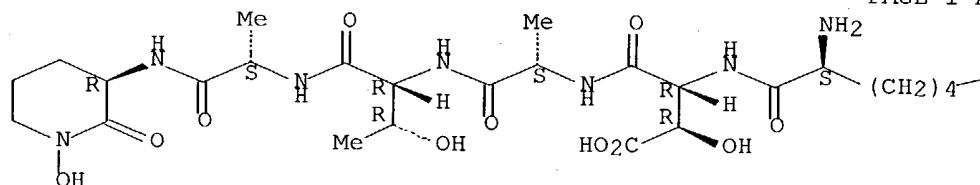
RL: SPN (Synthetic preparation); PREP (Preparation)
 (chromophore of, preparation of)

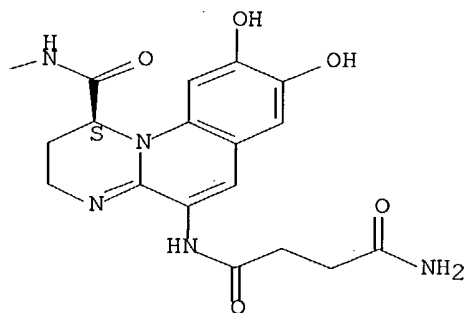
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L14 ANSWER 73 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:473258 CAPLUS Full-text

DN 113:73258

TI Purification, characterization, and structure of pseudobactin 589 A, a siderophore from a plant growth promoting *Pseudomonas*

AU Persmark, Magnus; Frejd, Torbjorn; Mattiasson, Bo

CS Chem. Cent., Univ. Lund, Lund, S-221 00, Swed.

SO Biochemistry (1990), 29(31), 7348-56

CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

AB Under conditions of low-Fe stress the plant growth-promoting bacterium *P. putida* 589 (DSM 50202) produced a yellow-green fluorescent Fe-binding peptide siderophore, which was designated pseudobactin 589 A and had an affinity constant toward Fe³⁺ of 1025 at pH 7. Protonated pseudobactin 589 A had the mol. formula C₅₄H₇₈O₂₆N₁₅ and a nominal mass spectral mol. mass of 1353 g/mol. Its structure was determined by a combination of NMR, fast atom bombardment mass spectrometry, and Edman degradation. Pseudobactin 589 A consisted of a nonapeptide with the amino acid sequence L-Asp-L-Lys-(D)-β-OH-Asp-D(L)-Ser-L-Thr-D-Ala-D-Glu-L(D)-Ser-L-Nδ-OH-Orn, in which lysine was amide bonded via the carboxy and the Nε-amino groups. A quinoline-derived chromophore was connected via an amide bond to the α-amino N of aspartic acid and an L-malamide residue was attached to the chromophore. The 3 bidentate Fe³⁺-binding ligands consisted of an o-dihydroxy aromatic group from the quinoline derivative, β-hydroxyaspartic acid, and an internally cyclized Nδ-hydroxyornithine. The structure of pseudobactin 589 A is unique but strikingly similar to that of other pseudobactin-type siderophores from other plant growth promoting and plant deleterious pseudomonads.

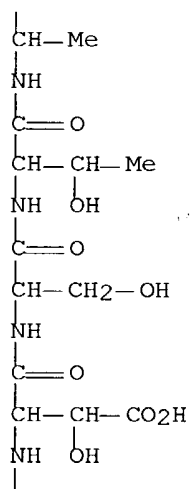
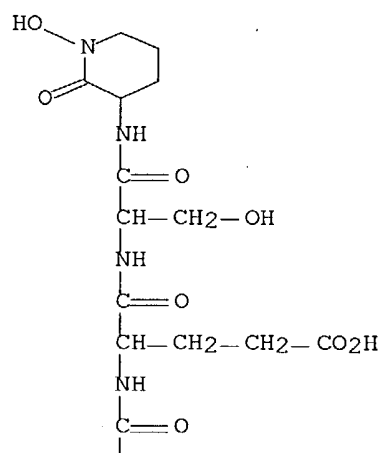
IT 128023-08-5P

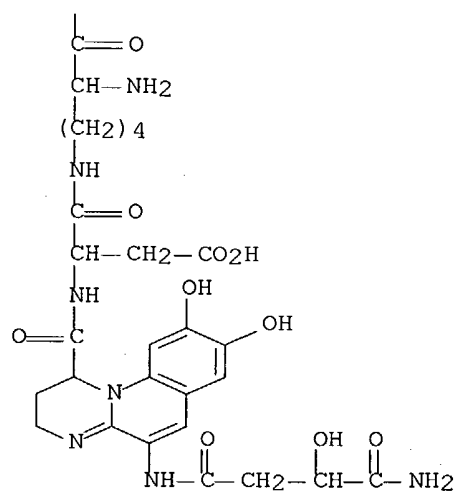
RL: PREP (Preparation)

(of *Pseudomonas putida*, purification and characterization and structure of)

RN 128023-08-5 CAPLUS

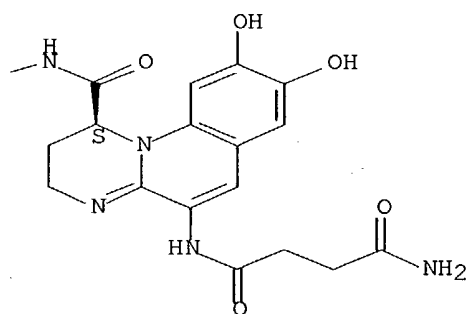
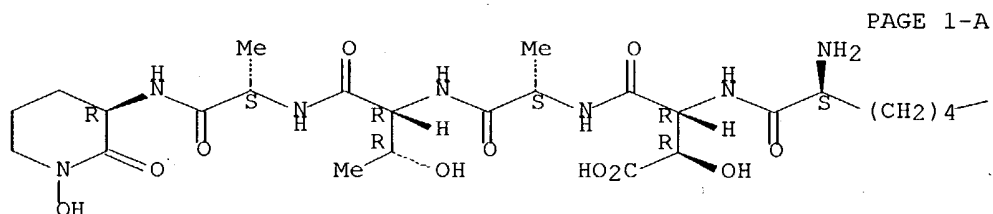
CN Serinamide, N6-[N-[[5-[(4-amino-3-hydroxy-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-α-aspartyl]-L-lysyl-threo-3-hydroxy-D-α-aspartylseryl-L-threonyl-D-alanyl-D-α-glutamyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1[S-(R*,R*)],7(S)]- (9CI) (CA INDEX NAME)





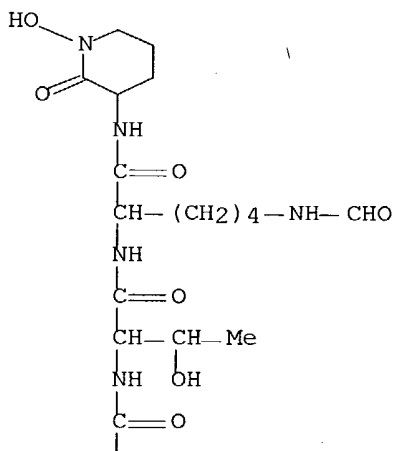
L14 ANSWER 74 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1989:633609 CAPLUS Full-text
 DN 111:233609
 TI Studies related to the syntheses of pseudobactin
 AU Kolasa, Teodozyj; Miller, Marvin J.
 CS Dep. Chem., Univ. Notre Dame, Notre Dame, IN, 46556, USA
 SO Pept.: Chem. Biol., Proc. Am. Pept. Symp. 10th (1988), Meeting Date
 1987,
 232-5. Editor(s): Marshall, Garland R. Publisher: ESCOM Sci. Pub.,
 Leiden, Neth.
 CODEN: 56MDA6
 DT Conference
 LA English
 AB A symposium.
 IT **76975-04-7P**, Pseudobactin
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (approaches toward the preparation of)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-
 D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

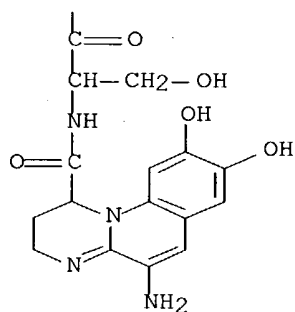
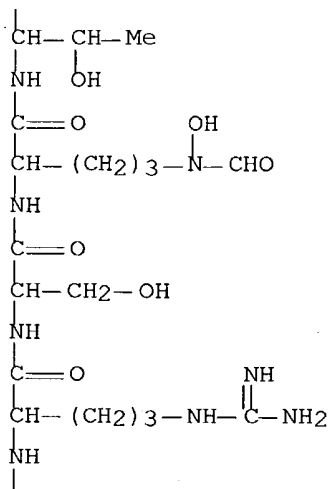
Absolute stereochemistry.



L14 ANSWER 75 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1989:473224 CAPLUS Full-text
 DN 111:73224
 TI Pseudomonas siderophores: structure and physicochemical properties of pyoverdins and related peptides
 AU Demange, P.; Wendenbaum, S.; Linget, C.; Bateman, A.; MacLeod, J.; Dell, A.; Albrecht, A. M.; Abdallah, M. A.
 CS Dep. Chim., Univ. Louis Pasteur, Strasbourg, 67000, Fr.
 SO Colloque INSERM (1989), 174 (Forum Pept., 2nd, 1988), 95-8
 CODEN: CINMDE; ISSN: 0768-3154
 DT Journal
 LA English
 AB Structure elucidation of the pyoverdins isolated from several strains of fluorescent pseudomonads belonging to different species has been accomplished using fast-atom bombardment mass spectrometry and high-resolution NMR. These siderophores consist of a peptide, constituted with 6-10 hydrophilic amino acids bound at its N terminus, to a chromophore derived from 2,3-diamino-6,7-dihydroxyquinoline.
 IT **121635-45-8D**, N-acyl derivs.
 RL: PROC (Process)
 (mol. structure determination of, of Pseudomonas aeruginosa)
 RN 121635-45-8 CAPLUS
 CN L-Lysinamide, N-[(5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl)carbonyl]-D-seryl-L-arginyl-D-seryl-N5-formyl-N5-hydroxy-L-ornithyl-L-threonyl-L-threonyl-N6-formyl-N-(1-hydroxy-2-oxo-3-piperidinyl)-, [1(S),7(S)]- (9CI) (CA INDEX NAME)

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IT 121613-10-3D, N-acyl derivs.

RL: PROC (Process)

(mol. structure determination of, of *Pseudomonas chlororaphis*)

RN 121613-10-3 CAPLUS

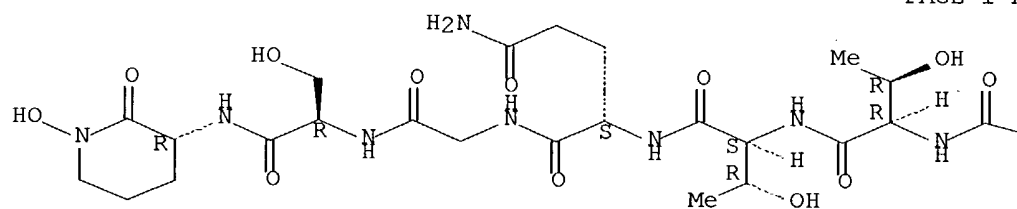
CN. Lysinamide, N-[(5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl)carbonyl]seryllsylglycyl-N5-hydroxyornithylseryl-N-(1-hydroxy-2-oxo-3-piperidiny)- (9CI) (CA INDEX NAME)

IT 121613-11-4D, N-acyl derivs. 121956-34-1D, N-acyl
derivs. 121986-85-4D, N-acyl derivs.
RL: PROC (Process)
(mol. structure determination of, of *Pseudomonas fluorescens*)
RN 121613-11-4 CAPLUS
CN D-Serinamide, N2-[[(1S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-
pyrimido[1,2-
a]quinolin-1-yl]carbonyl]-D-lysyl-N5-hydroxy-D-ornithylglycyl-D-
allothreonyl-L-threonyl-L-glutaminylglycyl-N-[(3R)-1-hydroxy-2-oxo-3-

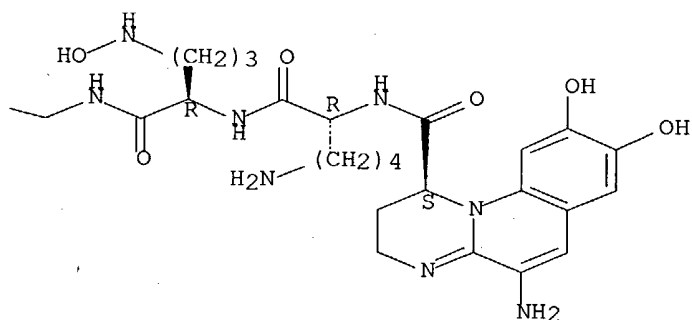
piperidiny]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

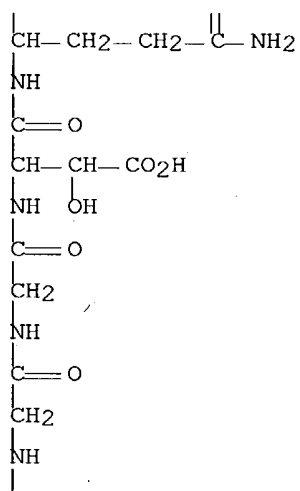
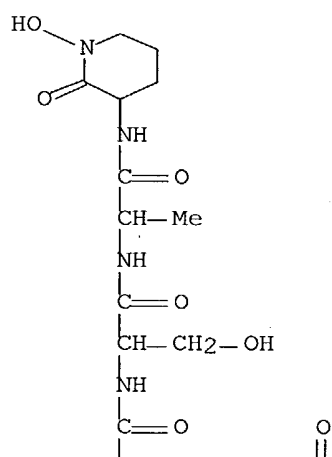
PAGE 1-A

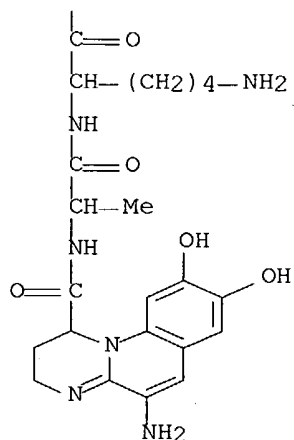


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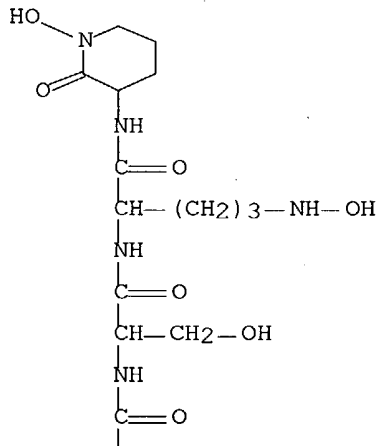
RN 121956-34-1 CAPLUS
CN Alaninamide, N-[(5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl)carbonyl]alanyllysylglycylglycyl-3-hydroxy-α-aspartylglutaminylseryl-N-(1-hydroxy-2-oxo-3-piperidiny)- (9CI) (CA INDEX NAME)

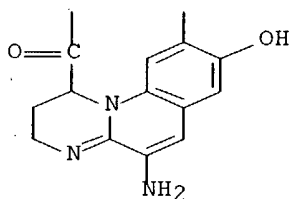
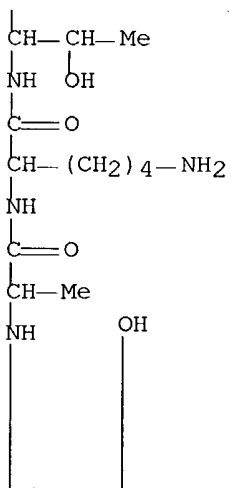




RN 121986-85-4 CAPLUS

CN Ornithinamide, N-[(5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl)carbonyl]alanyllysylthreonylseryl-N5-hydroxy-N-(1-hydroxy-2-oxo-3-piperidiny)- (9CI) (CA INDEX NAME)





IT 121613-08-9D, N-acyl derivs. 121986-84-3D, N-acyl derivs.

RL: PROC (Process)

(mol. structure determination of, of *Pseudomonas putida*)

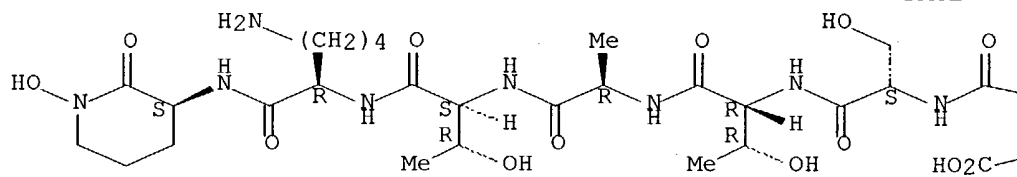
RN 121613-08-9 CAPLUS

CN D-Lysinamide, N-[[[(1S)-5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-

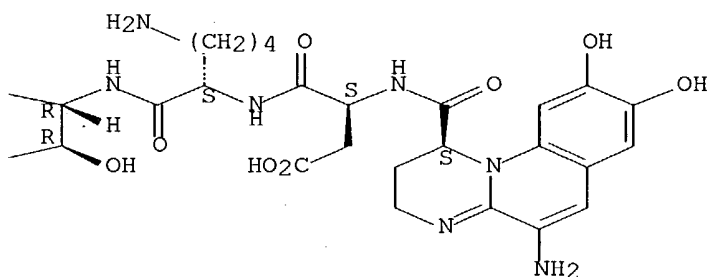
a]quinolin-1-yl]carbonyl]-L- α -aspartyl-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-seryl-D-allothreonyl-D-alanyl-L-threonyl-N-[(3S)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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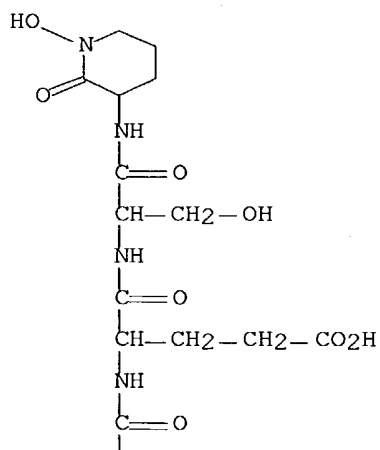


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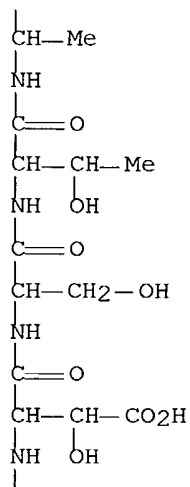


RN 121986-84-3 CAPLUS
 CN Serinamide, N-[(5-amino-2,3-dihydro-1H-pyrimido[1,2-a]quinolin-1-yl)carbonyl]-α-aspartyllysyl-3-hydroxy-α-aspartylserylthreonylalanyl-α-glutamyl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

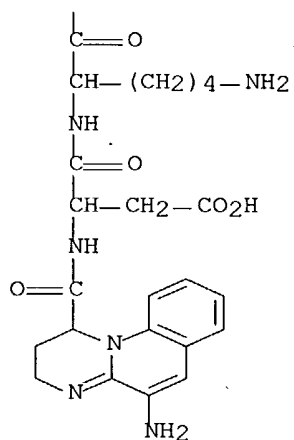
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IT 121613-09-0D, N-acyl derivs.

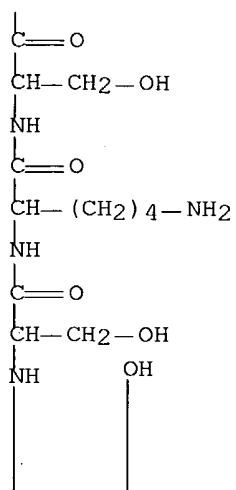
RL: PROC (Process)

(mol. structure determination of, of *Pseudomonas tolaasii*)

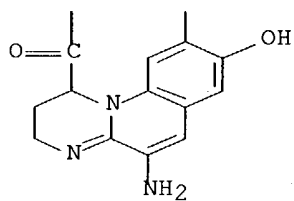
RN 121613-09-0 CAPLUS

CN Serinamide, N-[(5-amino-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl)carbonyl]seryllserylthreonylseryl-N5-hydroxyornithylthreonyl-N-(1-hydroxy-2-oxo-3-piperidinyl)- (9CI) (CA INDEX NAME)

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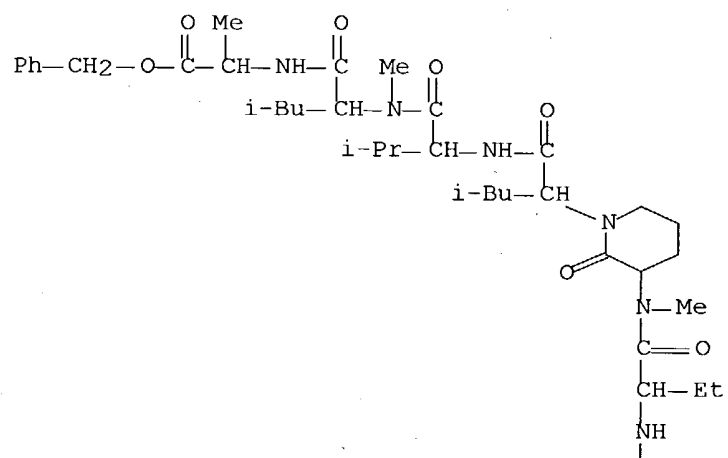


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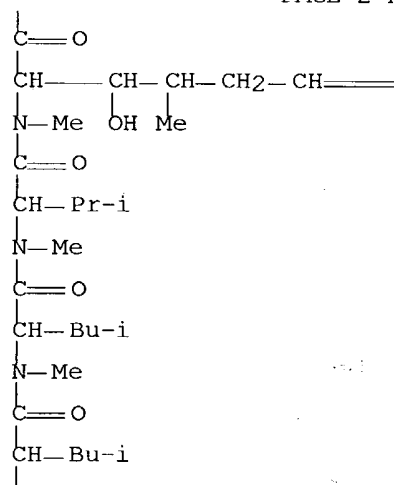


L14 ANSWER 76 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1988:570918 CAPLUS Full-text
 DN 109:170918
 TI Synthesis, conformation and immunosuppressive activity of a
 conformationally restricted cyclosporin lactam analog
 AU Aebi, Johannes D.; Guillaume, Dominique; Dunlap, Brian E.; Rich, Daniel
 H.
 CS Sch. Pharm., Univ. Wisconsin, Madison, WI, 53706, USA
 SO Journal of Medicinal Chemistry (1988), 31(9), 1805-15
 CODEN: JMCMAR; ISSN: 0022-2623
 DT Journal
 LA English
 OS CASREACT 109:170918
 AB Cyclosporin A (CsA, I), an immunosuppressive cyclic undecapeptide, in
 apolar solvent adopts a II' β -turn at the Sar3-MeLeu4 residues. [D-
 Proline3]Cs is a nonimmunosuppressive analog in which the II' β -turn is
 retained. In order to determine if this loss of activity is caused by
 steric hindrance between the Cs analog and its receptor or is caused by
 a change in the peptide conformation, an analog that stabilized a II' β -
 turn has been synthesized, [lactam3,4]Cs (II). The solution
 conformations of two other analogs, [D-MeAla3]Cs (III) and [L-MeAla3]Cs
 (IV), were also studied. The conformations have been established by ¹H
 NMR techniques. The conformations of II and III are indistinguishable
 from that of I in solution IV adopts a conformation with a cis amide
 bond between Sar3 and MeLU4. The inhibition of Con A stimulated
 thymocytes by I-IV gave IC50 values (nM) of 5, 100, 100, and 6, resp.
 The weak immunosuppressive activity of II possessing the II' β -turn
 suggests that the loss of activity is due to steric hindrance with the
 Cs receptor.
 IT **115160-84-4P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, deblocking, and cyclization of)
 RN 115160-84-4 CAPLUS
 CN L-Alanine, N-[(9H-fluoren-9-ylmethoxy)carbonyl]-D-alanyl-N-methyl-L-
 leucyl-N-methyl-L-leucyl-N-methyl-L-valyl-(2S,3R,4R,6E)-3-hydroxy-4-
 methyl-2-(methylamino)-6-octenoyl-(2S)-2-aminobutanoyl-(α S,3S)-3-
 (methylamino)- α -(2-methylpropyl)-2-oxo-1-piperidineacetyl-L-valyl-N-
 methyl-L-leucyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

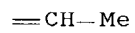
PAGE 1-A

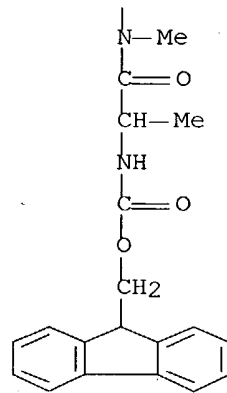


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PAGE 2-B

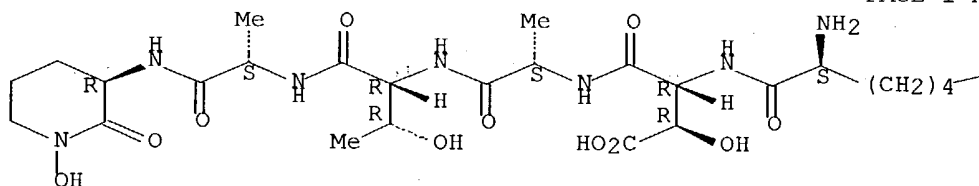




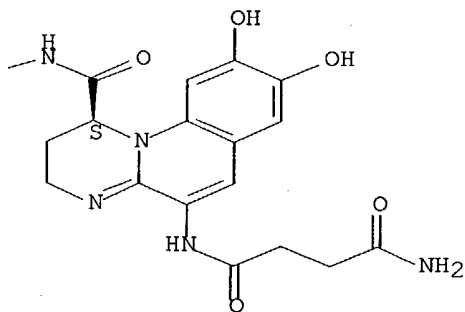
L14 ANSWER 77 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1987:594613 CAPLUS Full-text
 DN 107:194613
 TI Spectral properties of pseudobactin produced by *Pseudomonas* sp. B10
 AU MacDonald, James C.; Bock, Cheryl A.
 CS Plant Biotechnol. Inst., Natl. Res. Counc., Saskatoon, SK, S7N 0W9, Can.
 SO Canadian Journal of Botany (1987), 65(4), 703-5
 CODEN: CJBOAW; ISSN: 0008-4026
 DT Journal
 LA English
 AB The siderophore, pseudobactin, was isolated from the plant growth promoting rhizobacterium *Pseudomonas* B10, and its absorption and corrected fluorescence spectra were determined over a range of pH values. These spectra were similar to those reported for other fluorescent siderophores from other *Pseudomonas*, so that differentiation of pseudobactin from such related siderophores by absorption or fluorescence spectra is not feasible.
 IT **76975-04-7**, Pseudobactin
 RL: BIOL (Biological study)
 (of *Pseudomonas*, spectral properties of)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

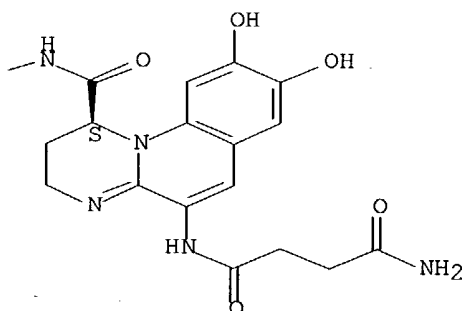
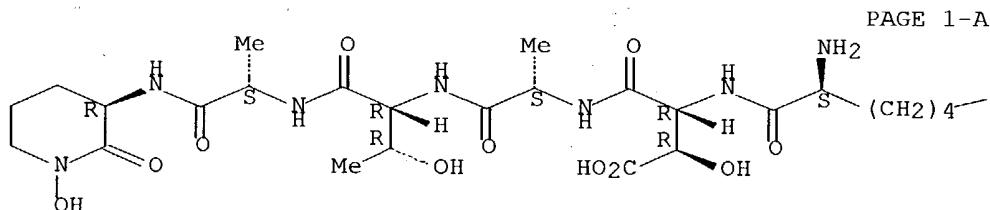


PAGE 1-B



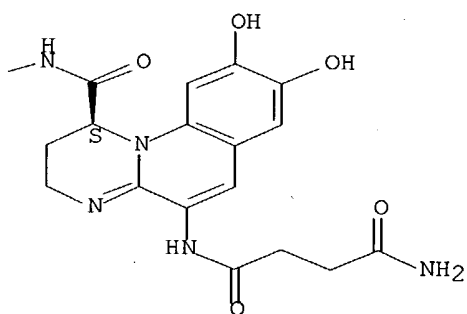
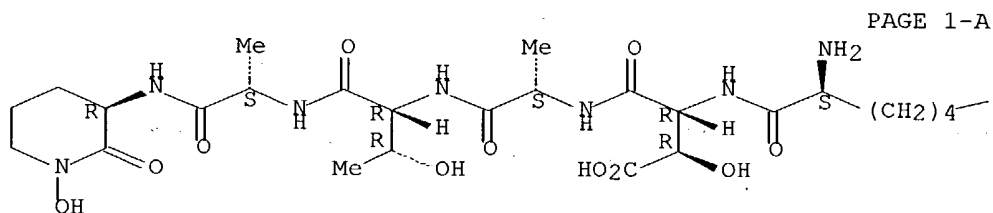
L14 ANSWER 78 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1987:550887 CAPLUS Full-text
 DN 107:150887
 TI Importance of siderophores in microbial interactions in the rhizosphere
 AU Loper, J. E.; Schroth, M. N.
 CS Dep. Plant Pathol., Univ. California, Berkeley, CA, 94720, USA
 SO NATO ASI Series, Series A: Life Sciences (1986), 117(Iron,
 Siderophores,
 Plant Dis.), 85-98
 CODEN: NALSDJ; ISSN: 0258-1213
 DT Journal; General Review
 LA English
 AB The role of siderophore production by pseudomonads in plant growth
 promotion and the control of certain diseases is considered, and factors
 affecting the efficacy of microbial antagonists are discussed.
 Pseudomonas Strains varied with respect to temperature range conducive
 to siderophore production and Fe-dependent growth. Sugars, amino acids,
 and organic acids commonly found in root exudates generally supported
 growth and fluorescent pigment/siderophore production by several
 beneficial Pseudomonas strains.
 IT **76975-04-7, Pseudobactin**
 RL: BIOL (Biological study)
 (Pseudomonas strains utilization of, temperature in relation to)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-
 D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 79 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1987:44987 CAPLUS Full-text
 DN 106:44987
 TI Iron assimilation genes from a plant growth-promoting *Pseudomonas* strain
 AU Moores, Jane C.; Magazin, Marilyn; Ditta, Gary S.; Leong, John
 CS Dep. Chem., Univ. California, San Diego, La Jolla, CA, 92093, USA
 SO Adv. Mol. Genet. Bact.-Plant Interact., Proc. Int. Symp., 2nd (1985),
 Meeting Date 1984, 205-6. Editor(s): Szalay, Aladar A.; Legocki, Roman
 P. Publisher: Boyce Thompson Inst. Plant Res., Ithaca, N. Y.
 CODEN: 55IDAD
 DT Conference
 LA English
 AB Progress toward cloning the gene encoding the putative outer membrane
 receptor for ferric pseudobactin [76975-04-7] in *Pseudomonas* B10 and
 characterization of its protein product is described.
 IT 76975-04-7D, iron complexes
 RL: PRP (Properties)
 (gene for receptor for, of *Pseudomonas*, cloning of)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-
 8,9-
 dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-
 hydroxy-
 D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-
 piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L14 ANSWER 80 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:478020 CAPLUS Full-text

DN 105:78020

TI The remedy of lime-induced chlorosis in peanuts by *Pseudomonas* sp. siderophores

AU Yurkevich, E.; Hadar, Y.; Chen, Y.

CS Fac. Agric., Hebrew Univ. Jerusalem, Rehovot, 76100, Israel

SO Journal of Plant Nutrition (1986), 9(3-7), 535-45

CODEN: JPNUDS; ISSN: 0190-4167

DT Journal

LA English

AB Siderophore-producing *Pseudomonas* strains were isolated from the rhizospheres of cotton (*Gossypium herbaceum*) and peanuts (*Arachis hypogaea*) (strains 1 and 11, resp.). Siderophores were produced in Fe-deficient culture medium. FeCl₃ was added to the culture media at the end of the growth period to produce an Fe-pigment complex. These solns. were applied to the soil directly or after removal of bacteria and free salts by centrifugation and dialysis. Peanuts grown in 0.5 kg pots on a highly calcareous soil (63% CaCO₃) and exhibiting severe Fe chlorosis were used to test the Fe-siderophore or Fe siderophore-bacteria activity as soil amendments for correcting Fe deficiency. The plants were treated with FeEDDHA (10 mg/500 g soil), Fe complexes with pigments from the 2 isolates, and bacterial suspension containing the Fe-pigment complex. Plants grown on untreated soil were used as a control. Significant increase of chlorophyll concentration of the treated plants was observed after 7 wk of growth in a growth chamber. Strain 1 was more efficient than strain 11 although both strains produced a similar amount of pigment. In both strains, the bacterial suspension was more effective than the separated Fe-pigment complex. DTPA-extractable Fe in soils treated with the various pigments was 2-fold that in the control and the FeEDDHA treatments. The pots were replanted with peanuts but were not treated with any addnl. Fe amendment. After 6 wk of growth, the chlorophyll content was higher in plants grown on the previously pigment-treated soils than in the FeEDDHA treated and control plants. Siderophore-producing bacteria may have a role in controlling lime-induced Fe deficiency in plants.

IT 76975-04-7

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(as soil amendment, for iron chlorosis correction)

RN 76975-04-7 CAPLUS

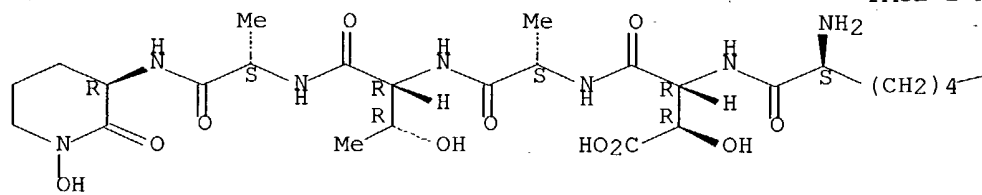
CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-

8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-

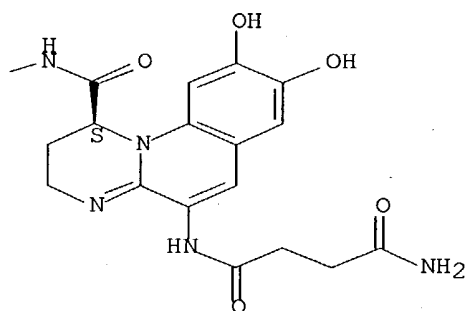
hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L14 ANSWER 81 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:103483 CAPLUS Full-text

DN 104:103483

TI Cloning of the gene coding for the outer membrane receptor protein for ferric pseudobactin, a siderophore from a plant growth-promoting *Pseudomonas* strain

AU Magazin, Marilyn D.; Moores, Jane C.; Leong, John

CS Dep. Chem., Univ. California, La Jolla, CA, 92093, USA

SO Journal of Biological Chemistry (1986), 261(2), 795-9

CODEN: JBCHA3; ISSN: 0021-9258

DT Journal

LA English

AB Plant growth-promoting *Pseudomonas* B10 produces its yellow-green, fluorescent siderophore (microbial iron transport agent) pseudobactin [76975-04-7] under iron-limiting conditions. A structural gene encoding the 85,000-dalton (Da) putative outer membrane receptor protein for ferric pseudobactin was identified in a gene bank from *Pseudomonas* B10 prepared with the broad-host-range conjugative cosmid cloning vector pLAFR1. Transposon Tn5 mutagenesis of recombinant plasmid pJLM300 localized the functional gene to a region of .apprx.2.4 kilobases, consistent with the apparent mol. weight of the receptor protein. Mobilization of pJLM300 into *Pseudomonas* A124 and A225, whose growth was inhibited by *Pseudomonas* B10 or pseudobactin, rendered these strains no longer susceptible to iron starvation by pseudobactin because they were now able to transport ferric pseudobactin. Pseudobactin biosynthetic genes flanked this receptor gene on both sides and were on sep. operons. Transposon Tn5 insertion mutants of *Pseudomonas* B10 lacking this receptor protein were generated by a marker exchange technique and were defective in ferric pseudobactin transport. Such mutants could be complemented in trans by pJLM300. The production of pseudobactin, the receptor protein, and 4 other outer membrane proteins in *Pseudomonas* B10 was coordinately regulated by the level of intracellular iron.

IT 76975-04-7

RL: PRP (Properties)

(gene for, of plant growth-promoting *Pseudomonas*, cloning and insertion mutagenesis of)

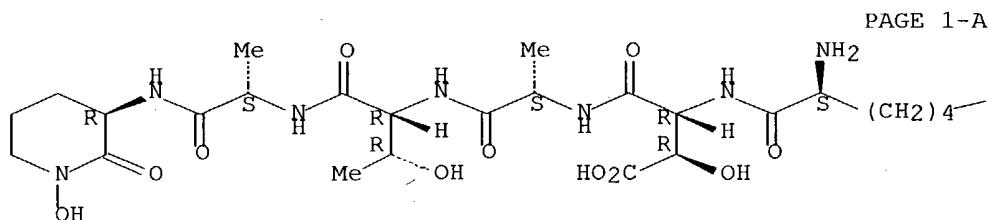
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-

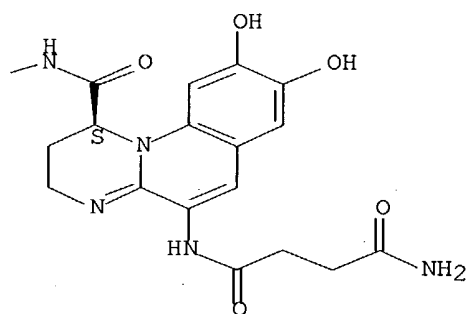
dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-

D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

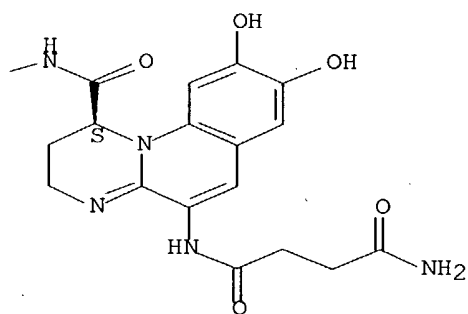
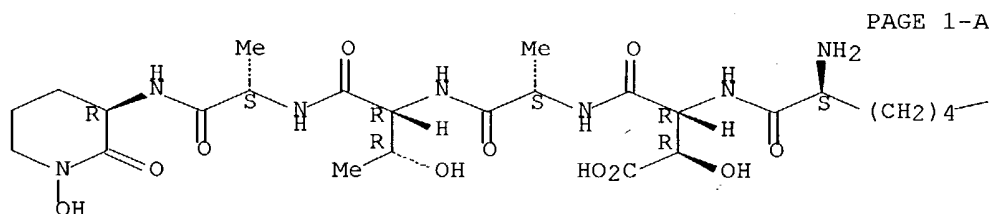


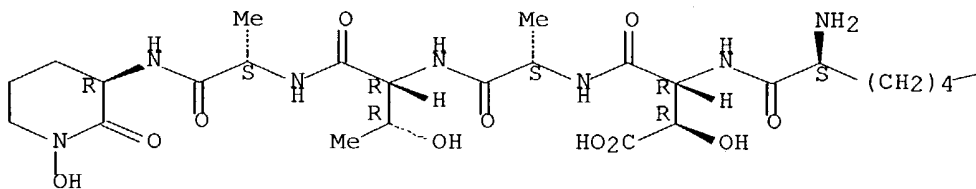
PAGE 1-B

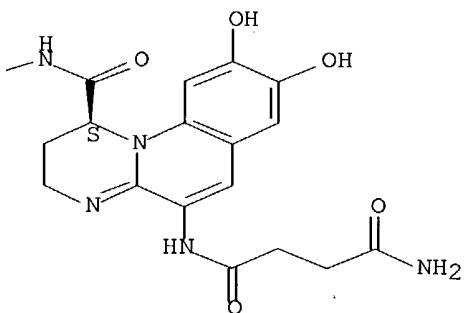


L14 ANSWER 82 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1985:403980 CAPLUS Full-text
 DN 103:3980
 TI Inhibitory effect of pseudobactin on the uptake of iron by higher plants
 AU Becker, J. O.; Hedges, R. W.; Messens, E.
 CS Lab. Histol., Rijksuniv. Gent, Ghent, B-9000, Belg.
 SO Applied and Environmental Microbiology (1985), 49(5), 1090-3
 CODEN: AEMIDF; ISSN: 0099-2240
 DT Journal
 LA English
 AB Purified pseudobactin inhibits the uptake of FeCl₃ by the roots of pea and maize sufficiently to reduce the synthesis of chlorophyll. This inhibition is interpreted as competitive binding, as described for synthetic chelating compds.
 IT **76975-04-7**
 RL: BIOL (Biological study)
 (iron uptake inhibition by, in pea and corn)
 RN 76975-04-7 CAPLUS
 CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

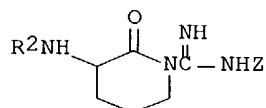
Absolute stereochemistry.







L14 ANSWER 84 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1983:34930 CAPLUS Full-text
 DN 98:34930
 TI Synthesis of leupeptins and inhibitory studies of proteases
 AU Borin, Gianfranco; Chessa, Gavino; Marchiori, Fernando; Mueller-Esterl, Werner
 CS Cent. Studi Biopolimeri, CNR, Padua, Italy
 SO Pept., Proc. Eur. Pept. Symp., 16th (1981), Meeting Date 1980, 435-40.
 Editor(s): Brunfeldt, K. Publisher: Scriptor, Copenhagen, Den.
 CODEN: 48NWA3
 DT Conference
 LA English
 GI



II

AB Leupeptins R-Leu-Leu-Arg-H [I; R = Ac, EtCO, H, Me3CO2C (Boc), CF3CO; Arg-H = argininal] were prepared by coupling R1-Leu-Leu-OH [R1 = Ac, EtCO, PhCH2O2C (Z), Boc, CF3CO] with lactam II (R2 = H) by DCC/hydroxysuccinimide, reducing the resulting II [R2 = R1-Leu-Leu], and deblocking the resulting R1-Leu-Leu-Arg(Z)-H by hydrogenolysis. Boc-Arg(Z)-OH was cyclized by ClCO2CH2CHMe2 to give II (R2 = Boc), which was Boc-deblocked to give II (R2 = H). I (R = Ac, EtCO, Boc) were also prepared by stepwise couplings with II (R2 = H) and Boc-Leu-ONSu (NSu = succinimido). The inhibitory capacity of I against trypsin and acrosin decreased in the following order of R: Boc > Ac > EtCO > CF3CO » H and Boc > CF3CO, EtCO > Ac » H, resp.

IT 40610-83-1P 81344-51-6P 81344-52-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT

(Reactant or reagent)

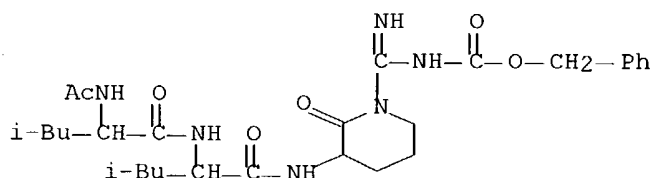
(preparation and hydride reduction of)

RN 40610-83-1 CAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[1-

[imino[[(phenylmethoxy) carbonyl] amin

o]methyl]-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)

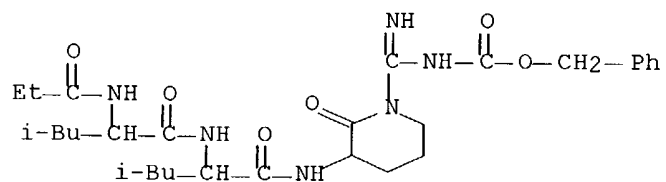


RN 81344-51-6 CAPLUS

CN L-Leucinamide, N-(1-oxopropyl)-L-leucyl-N-[1-

[imino[[(phenylmethoxy) carbon

yl]amino]methyl]-2-oxo-3-piperidiny]-, (S)- (9CI) (CA INDEX NAME)

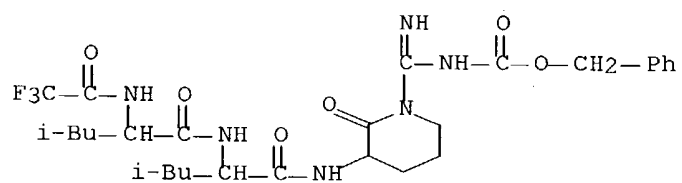


RN 81344-52-7 CAPLUS

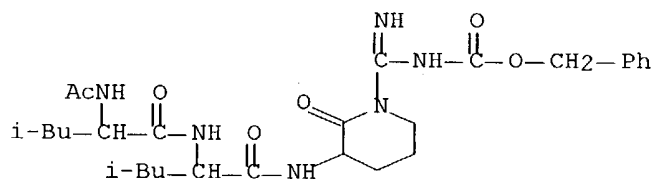
CN L-Leucinamide, N-(trifluoroacetyl)-L-leucyl-N-[1-
[imino[[(phenylmethoxy) carbonyl] amino]methyl]-2-oxo-3-piperidinyl]-,

(S)-

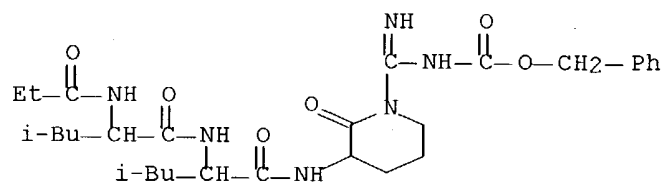
(9CI) (CA INDEX NAME)



L14 ANSWER 85 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1982:174592 CAPLUS Full-text
 DN 96:174592
 TI Synthesis of leupeptins and inhibition of proteinases. I. Inhibition
 of
 acrosin and trypsin
 AU Borin, Gianfranco; Chessa, Gavino; Cavaggion, Gianfranco; Marchiori,
 Fernando; Mueller-Esterl, Werner
 CS Ist. Chim. Org., Univ. Padova, Padua, 35100, Italy
 SO Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie (1981), 362(11),
 1435-45
 CODEN: HSZPAZ; ISSN: 0018-4888
 DT Journal
 LA English
 AB A series of leupeptin analogs R-L-leucyl-L-leucyl-L-argininal with
 variable N-terminal substituents were synthesized using N α -tert-
 butyloxycarbonyl-NG-benzyloxycarbonyl-L-arginine- δ -lactam [51219-20-6]
 as the starting material. The modified leupeptins were strong
 competitive inhibitors of the endoprotease acrosin [9068-57-9] from
 mammalian spermatozoa. Inhibition consts. were in the range $4.7 + 10^{-7}$
 M (R = H)- $9.7 + 10^{-9}$ M (R = tert-butyloxycarbonyl). N α -tert-
 butyloxycarbonyl leupeptin [81344-47-0] Represents the strongest acrosin
 inhibitor synthesized so far. Two of the leupeptin derivs. (R =
 trifluoroacetyl, R = tert-butyloxycarbonyl) were more effective than the
 natural leupeptins from microbial sources ($K_i = 5.9 + 10^{-8}$ M). The
 potential use of synthetic leupeptins as antienzymic contraceptives is
 discussed.
 IT **40610-83-1P 81344-51-6P 81344-52-7P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT
 (Reactant or reagent)
 (preparation and deprotection of)
 RN 40610-83-1 CAPLUS
 CN L-Leucinamide, N-acetyl-L-leucyl-N-[1-
 [imino[[(phenylmethoxy) carbonyl] amin
 o]methyl]-2-oxo-3-piperidiny]- (9CI) (CA INDEX NAME)



RN 81344-51-6 CAPLUS
 CN L-Leucinamide, N-(1-oxopropyl)-L-leucyl-N-[1-
 [imino[[(phenylmethoxy) carbon
 yl]amino]methyl]-2-oxo-3-piperidiny]-, (S)- (9CI) (CA INDEX NAME)

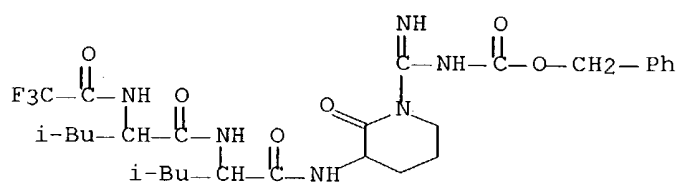


RN 81344-52-7 CAPLUS

CN L-Leucinamide, N-(trifluoroacetyl)-L-leucyl-N-[1-
[imino[[(phenylmethoxy) carbonyl] amino]methyl]-2-oxo-3-piperidinyl]-,

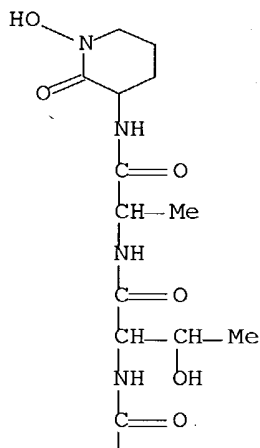
(S)-

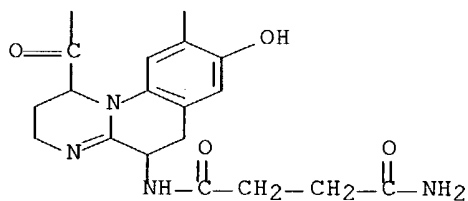
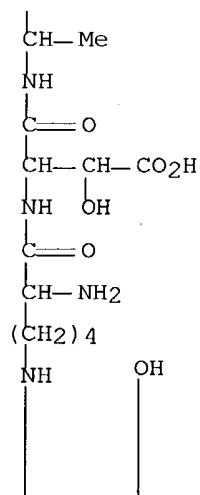
(9CI) (CA INDEX NAME)



L14 ANSWER 86 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 1981:565217 CAPLUS Full-text
 DN 95:165217
 TI Structure of pseudobactin A, a second siderophore from plant growth promoting *Pseudomonas* B10
 AU Teintze, Martin; Leong, John
 CS Dep. Chem., Univ. California, La Jolla, CA, 92093, USA
 SO Biochemistry (1981), 20(22), 6457-62
 CODEN: BICHAW; ISSN: 0006-2960
 DT Journal
 LA English
 AB The structure of nonfluorescent pseudobactin A, one of 2 extracellular siderophores (microbial Fe transport agents) produced by the plant growth-promoting bacterium *Pseudomonas* B10, was determined by comparison of its ¹H and ¹³C NMR spectra with those of yellow-green, fluorescent pseudobactin, the other siderophore. The only structural difference between pseudobactin and pseudobactin A was that the latter was saturated at carbons 3 and 4 of the quinoline derivative, whereas pseudobactin is unsatd. at these positions. A mechanism is proposed for the observed conversion of pseudobactin A into pseudobactin in aqueous solution
 IT **79438-64-5**
 RL: PROC (Process) (of *Pseudomonas*, structure determination of)
 RN 79438-64-5 CAPLUS
 CN L-Alaninamide, N6-[[5-[(4-amino-1,4-dioxobutyl)amino]-2,3,5,6-tetrahydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-(1-hydroxy-2-oxo-3-piperidiny)- (9CI) (CA INDEX NAME)

PAGE 1-A





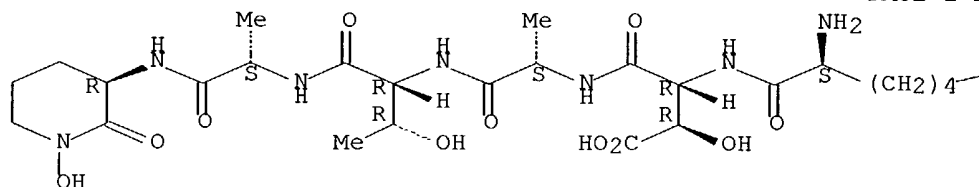
IT 76975-04-7

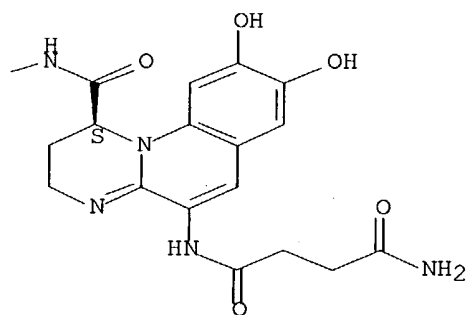
RL: BIOL (Biological study)
 (pseudobactin A in relation to)

RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[(1S)-5-[(4-amino-1,4-dioxobutyl) amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl] carbonyl]-L-lysyl-(3R)-3-hydroxy-D-α-aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidiny]- (9CI). (CA INDEX NAME)

Absolute stereochemistry.





L14 ANSWER 87 OF 89 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1981:564158 CAPLUS Full-text

DN 95:164158

TI Structure of ferric pseudobactin: a siderophore from a plant growth promoting *Pseudomonas*

AU Teintze, Martin; Hossain, M. B.; Barnes, C. L.; Leong, John; Van der Helm, Dick

CS Dep. Chem., Univ. California, La Jolla, CA, 92093, USA

SO Biochemistry (1981), 20(22), 6446-57

CODEN: BICHAW; ISSN: 0006-2960

DT Journal

LA English

AB The structure of the title compound was determined by single-crystal x-ray diffraction methods using counter data. The structure consisted of linear hexapeptide, L-Lys-D-threo- β -OH-Asp-L-Ala-D-allo-Thr-L-Ala-D-N δ -OH-Orn, in which the N δ -OH nitrogen of the ornithine was cyclized with the C-terminal carboxyl group, and the Ne-amino group of the lysine was linked via an amide bond to a fluorescent quinoline derivative. The Fe chelating groups consisted of a hydroxamate group derived from N δ -hydroxyornithine, an α -hydroxy acid derived from β -hydroxyaspartic acid, and an o-dihydroxy aromatic group derived from the quinoline moiety. Pseudobactin crystallized as a single coordination isomer with the Λ absolute configuration. In the crystal structure, ferric pseudobactin formed a dimer, which constituted the asym. unit. The asym. unit also contained 26 water mols. The mols. in the dimer were related by a pseudo-2-fold sym. axis. Red-brown crystals of ferric pseudobactin (C₄₂H₅₇N₁₂O₁₆Fe·13H₂O), obtained from pyridine-AcOH buffer solution equilibrated with water, conformed to space group I2 with a = 29.006, b = 14.511, c = 28.791 Å, and β = 96.06° at -135°. For 8 mols./unit cell, the calculated d. was 1.38 g/cm³; the observed d. was 1.40 g/cm³. The structure was refined by least-squares methods with anisotropic thermal parameters for all nonhydrogen atoms to a final R factor of 0.08.

IT 76975-04-7

RL: PROC (Process)

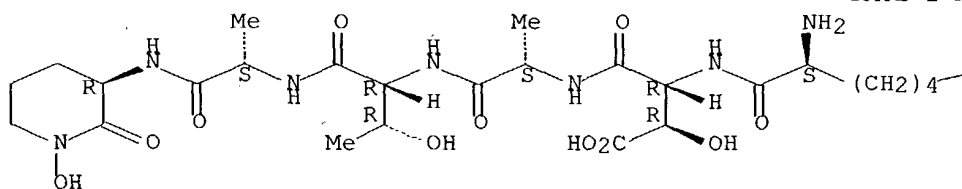
(of *Pseudomonas*, structure determination of)

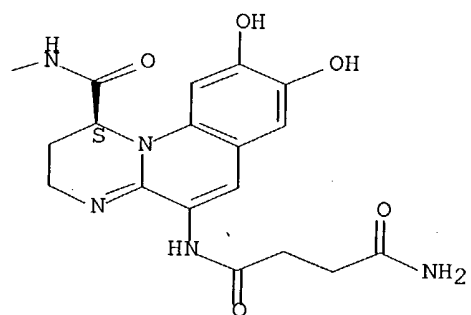
RN 76975-04-7 CAPLUS

CN L-Alaninamide, N6-[[[(1S)-5-[(4-amino-1,4-dioxobutyl)amino]-2,3-dihydro-8,9-dihydroxy-1H-pyrimido[1,2-a]quinolin-1-yl]carbonyl]-L-lysyl-(3R)-3-hydroxy-D- α -aspartyl-L-alanyl-D-allothreonyl-N-[(3R)-1-hydroxy-2-oxo-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



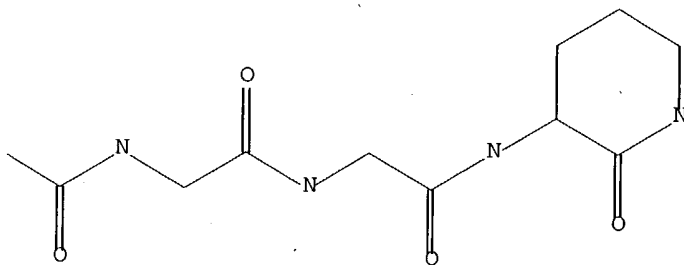


PAGE 1-B

=> d 11; d 14; d 17; d 19; d 111; d his; log y

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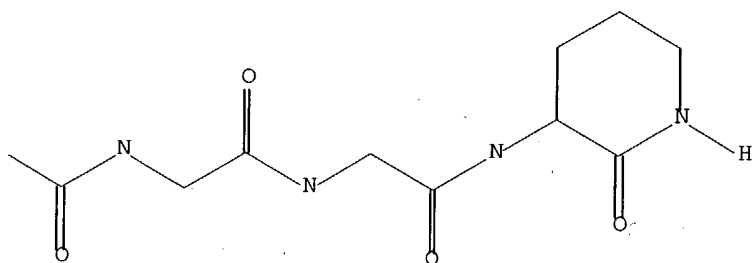
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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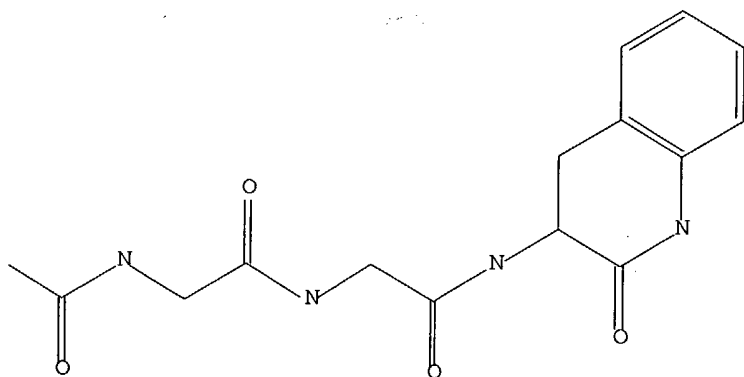
L4 STR



Structure attributes must be viewed using STN Express query preparation.

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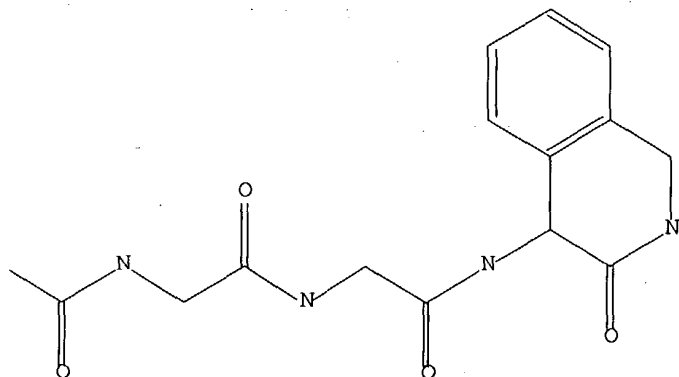
L7 STR



Structure attributes must be viewed using STN Express query preparation.

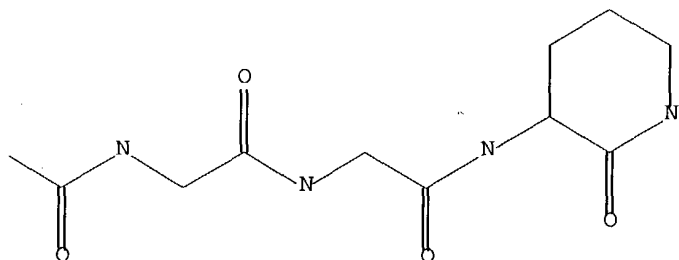
L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

L11 HAS NO ANSWERS
L11 STR



Structure attributes must be viewed using STN Express query preparation.

(FILE 'HOME' ENTERED AT 18:54:47 ON 15 SEP 2004)

FILE 'REGISTRY' ENTERED AT 18:55:12 ON 15 SEP 2004

L1 STRUCTURE UPLOADED
L2 7 S L1
L3 144 S L1 FUL

FILE 'STNGUIDE' ENTERED AT 18:55:32 ON 15 SEP 2004

FILE 'REGISTRY' ENTERED AT 18:56:09 ON 15 SEP 2004

L4 STRUCTURE UPLOADED
L5 9 S L4 FUL SUB=L3
L6 135 S L3 NOT L5
L7 STRUCTURE UPLOADED
L8 4 S L7 FUL SUB=L6
L9 STRUCTURE UPLOADED
L10 0 S L9 FUL SUB=L6
L11 STRUCTURE UPLOADED
L12 78 S L11 FUL SUB=L6
L13 82 S L8 OR L12

FILE 'CAPLUS' ENTERED AT 19:02:05 ON 15 SEP 2004

L14 89 S L13

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

421.54

728.03

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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-60.90

STN INTERNATIONAL LOGOFF AT 19:03:23 ON 15 SEP 2004